

# 13<sup>th</sup> INTERNATIONAL CONFERENCE ON QUASICRYSTALS

(ICQ13)



**18-23 September 2016**

**Kathmandu, Nepal**

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NRNA: Dr Upendra Mahato-Dr Shesh Ghale-Jiba Lamichhane-Bhaban Bhatta-Kumar Panta-Ram Thapa-Dr Badri KC-Kul Acharya-Dr Ambika Adhikari

Dear friends and colleagues,

Namaste and Welcome to the 13<sup>th</sup> International Conference on Quasicrystals (ICQ13) being held in Kathmandu, the capital city of Nepal.

This episode of conference on quasicrystals follows twelve previous successful meetings held at cities Les Houches, Beijing, Vista-Hermosa, St. Louis, Avignon, Tokyo, Stuttgart, Bangalore, Ames, Zürich, Sapporo and Cracow. Let's continue with our tradition of effective scientific information sharing and vibrant discussions during this conference. The research on quasicrystals is still evolving. There are many physical properties waiting for scientific explanation, and many new phenomena waiting to be discovered. In this context, the conference is going to cover a wide range of topics on quasicrystals such as formation, growth and phase stability; structure and modeling; mathematics of quasiperiodic and aperiodic structures; transport, mechanical and magnetic properties; surfaces and overlayer structures. We are also going to have discussion on other aspects of materials science, for example, metamaterials, polymer science, macro-molecules system, photonic/phononic crystals, metallic glasses, metallic alloys and clathrate compounds.

Nepal is home to eight of ten highest mountains in the world are located in Nepal, which include the world's highest, Mt Everest (SAGARMATHA). Nepal is also famous for cultural heritages. It houses ten UNESCO world heritage sites, including the birth place of the Lord Buddha, Lumbini. Seven of the sites are located in Kathmandu valley itself. We hope you will have opportunity to explore this small but diverse country.

As we are all aware that Nepal was shaken very badly by two big earthquakes last year. More than eight thousand people lost their lives, and many more were injured. Nepal had to bear a huge loss of infrastructure and financial resources of the scale never seen in its long history. Many cultural and ancient historical sites were crumbled apart in the Kathmandu valley by this natural disaster. But we are glad to share with you all that the inimitable natural beauty of Nepal and hospitality of Nepali people are unaltered. Nepal is going through a long and slow recovery process, and it will be a long time before reconstruction will be completed. Your visit to Kathmandu during this difficult time means a lot to Nepal and her people. It will help to send a message to the world that Nepal is still a safe place to visit. We strongly believe that local universities and researchers will benefit from the conference.

We thank Prof Dan Shechtman (the 2011 Nobel Laureate in Chemistry), invited speakers and all other participants for their valuable scientific contribution. Thanks also go to all sponsors. We gratefully acknowledge the support for the conference from the University of Liverpool, UK, Tohoku University, Japan and Tribhuvan University, Nepal. We are honoured by the presence of officials from Nepal government, Tribhuvan University, Kathmandu University in the inauguration ceremony.

We wish you a memorable stay at the historic and cultural center of the Himalayan country, and look forward to your future visits as well.

Chairs,

Dr Hem Raj Sharma (the University of Liverpool, UK)

Prof An Pang Tsai, Tohoku University, Japan

Local organising committee chair

Prof Narayan P Adhikari, Tribhuvan University, Kathmandu, Nepal



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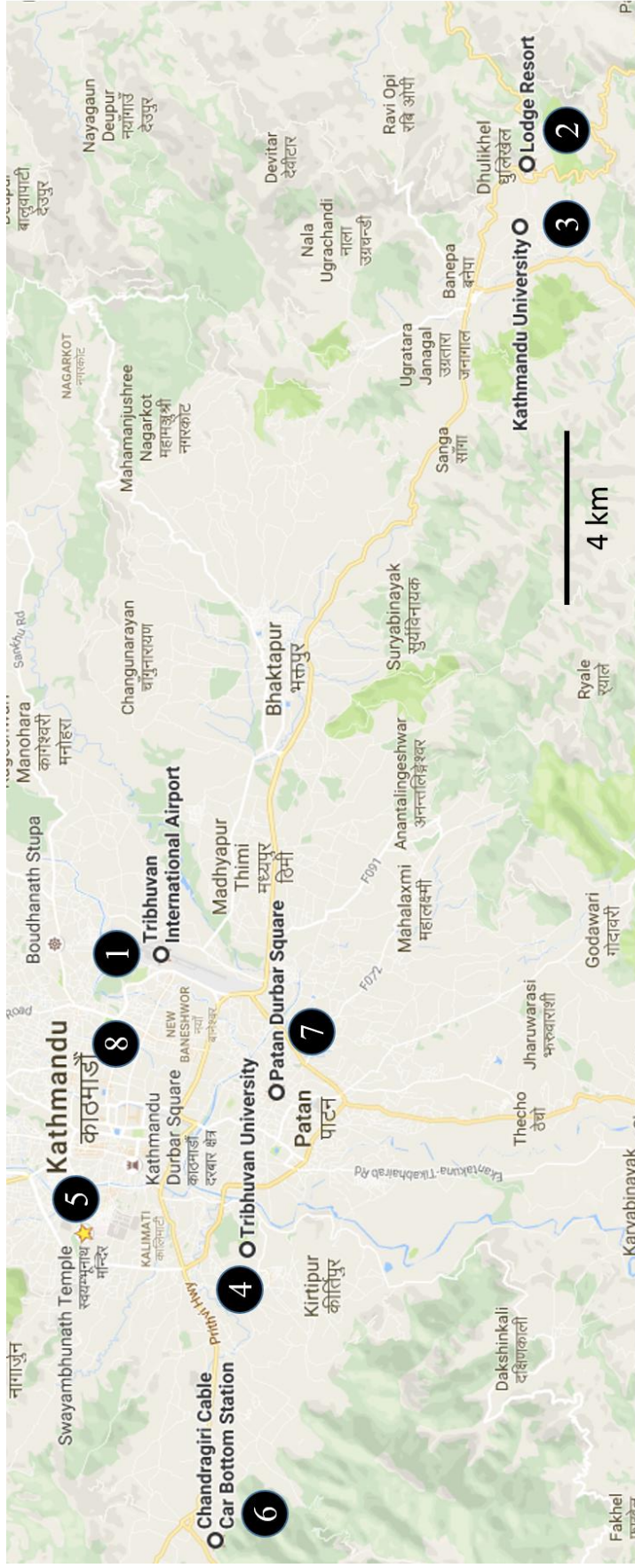
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# Useful Information

## **Contact Phone Numbers**

Dhulikhel Lodge Resort (conference hotel): +977-11-490114, 490494, 490043

Dr Hem Raj Sharma/Prof An Pang Tsai (conference chairs):+977-9841668411

Prof Dr Narayan Adhikari (local organizing committee chair): +977-9841500796

Nepal Police Emergency number: +977-1-4228435

## **Conference Venue and Local Transportation**

The conference will be held in Dhulikhel Lodge Resort, which is about 30 km from Tribhuvan International Airport, Kathmandu. The tutorial on 18th will be hosted by Kathmandu University, which is located about 3 km from the Resort. The public lecture on 21st will be hosted by the Tribhuvan University Central Campus, which is about 30 km from the resort. The transportation from the airport to the resort, the resort to the Kathmandu University and Tribhuvan University will be arranged by the conference organizer. The participants are requested to confirm their time of arrival with flight details to the organizer in advance. Transportation to Kathmandu from Dhulikhel on other occasions can be provided by the hotel, but there will be a charge.

## **Poster Presentation**

The size of poster is A0 portrait (W: 841 mm x H: 1189 mm). Posters can be hanged in the designated area from Monday morning, and should be removed by Friday morning. Odd numbered posters should be presented on Monday, and even numbered on Tuesday.

## **Best Presentation Awards**

European C-MAC awards will be given for best presentations by young scientists (one award for poster and one for oral presentation).

## **Lunch and Dinner**

Lunch, dinner and welcome dinner will be provided at Dhulikhel Lodge Resort. Meal coupons will be provided with the conference kit. Participants will have to present a coupon at the meal time.

## **Public Lecture, Excursion and Conference Dinner**

Excursion and conference dinner will be held on 21<sup>st</sup>, following a public lecture by Daniel Shechtman in Tribhuvan University, Kirtipur. All participants, including accompanying persons, will leave Dhulikhel Lodge Resort at 10:10 am, for the public lecture. Accompanying persons may visit a historic area of Kirtipur during the public lecture. After the public lecture, participants will join the excursion.

For the excursion, participants may choose either Patan Durbar Square (world heritage site) or Chandragiri Hill top by cable car (panoramic views of Kathmandu Valley & Himalayan ranges from Annapurna to Everest). Participants should register the excursion at the registration desk. Conference dinner takes place in Bhojan Griha, Dillibazar, Kathmandu (+ 977-1- 4416423 / 4411603)

### **Program for Accompanying Persons and Post Conference Tours**

We have arranged a special programme for accompanying persons. We also offer post conference tours for participants who are interested in exploring the nature and history of Nepal. The tours start on Friday (23rd) and end on Sunday or Monday. Four different options are available.

OPTION 1: HERITAGE TRAVEL AND MOUNTAIN FLIGHT

OPTION 2: TREKKING, RAFTTING & EVEREST PACKAGE

OPTION 3: POKHARA TRAVEL

OPTION 4: JUNGLE SAFARI TRAVEL

Further details of the tours and activities for accompanying persons are provided in separate sheets. You can book the activities for accompanying persons and post conference tours at the registration desk or by sending an e-mail to DLR, [dlrdhuli@gmail.com](mailto:dlrdhuli@gmail.com) and copying it to [icq13@liverpool.ac.uk](mailto:icq13@liverpool.ac.uk). You can pay DLR for these activities after your arrival at the registration desk.

### **Currency**

Currency of Nepal is Nepalese Rupees, NRs (1 USD ~ NRs 106). You can exchange foreign currencies to NRs at the airport or conference hotel. You can withdraw NRs using VISA card in ATM machines available at the airport or city centre.



# Committees

## Conference Chairs

Dr. Hem Raj Sharma  
(The University of Liverpool, UK)  
Prof. An Pang Tsai  
(Tohoku University, Japan)

## Conference Secretary

Ms. Noriko Yubuta  
(Tohoku University, Japan)

## International Advisory Board

Michael Baake (Germany)  
Marc de Boissieu (France)  
Janez Dolinšek (Slovenia)  
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Walter Steurer (Switzerland)  
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Michael Widom (USA)  
Janusz Wolny (Poland)

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Ron Lifshitz (Israel)  
Hem Raj Sharma (UK)  
An Pang Tsai (Japan)

## Local Organising Committee

Chair: Prof. Narayan Prasad Adhikari  
(Central Department of Physics, TU)

### Members:

Prof. Amar Yadav (Central  
Department of Physics, TU)  
Dr. Rajendra Parajuli (Amrit Science  
Campus)  
Dr. Gopi Chandra Kafle (Central  
Department of Physics, TU)  
Dr. Lila Pradhan Joshi (Amrit Science  
Campus)  
Dr. Raju Adhikari (Nepal Science  
Foundation (NSF) and CSIRO  
Manufacturing, Australia)

# Invited Speakers

D. Shechtman (Nobel Laureate), Israel

E. Abe, Japan

S. Ben-Abraham, Israel

T. Dotera, Japan

E. Gaudry, France

A. Goldman, USA

A. Jagannathan, France

P. Jana, India

A. Julien, Norway

O. Perez, France

W. Steurer, Switzerland

N. Takemori, Japan

R. Widmer, Switzerland

# Program Overview

	Sunday 18th	Monday 19th	Tuesday 20th	Wednesday 21st	Thursday 22nd	Friday 23rd	Sat-Sun 24-25th
06:00 07:00		Morning walk tour/yoga					
		Breakfast	Breakfast	Breakfast	Breakfast	Breakfast	
07:00 09:00				Session IX			
08:40 09:00							
09:00 09:15							
09:15 09:20		Session I					
09:20 09:50	Registration open		Session V		Session X	Session XIV	
09:50 10:10	(Venue: DLR)						
10:10 10:30				Move to			
10:30 10:50		Coffee	Coffee	Tribhuvan	Coffee	Coffee	
10:50 11:20		Session II	Session VI	Tribhuvan	Session XI		
11:20 11:40	Tutorial 1			University			
11:40 12:00	(Venue: KU)			Shechtman's			
12:00 12:20				lecture		Lunch	
12:20 12:40	Tutorial 2		Lunch	in TU	Lunch	End	
12:40 13:00	(Venue: KU)						
13:00 13:10		Lunch		Lunch	Lunch		
13:10 13:40							
13:40 14:10	Refreshment			Excursion			
14:10 14:20	Tutorial 3				Session XII		
14:20 14:50	(Venue: KU)	Session III	Session VII				
14:50 15:10							
15:10 15:30	Move to						
15:30 15:40	conference						
15:40 15:50	hotel, DHL						
15:50 16:00		Coffee	Coffee				
16:00 16:20	Opening				Coffee		
16:20 16:40	ceremony	Session IV	Session VIII		Session XIII		
16:40 17:00	(Venue: DLR)						
17:00 17:20							
17:20 17:40		Break					
17:40 17:50			Break				
17:50 18:00		Poster	Poster		Break		
18:00 18:15		session with	session				
18:15 20:00	Welcome	dinner	with dinner	Conference			
20:00 21:00	dinner	Cultural	Cultural	dinner	Cultural		
	(Venue: DLR)	program	program		program		

Session I: Formation and Growth  
 Session II, III: Structure and Modeling  
 Session IV: Electronic Properties  
 Session V, VI: Transport Properties  
 Session VII: Magnetic Properties  
 Session VIII: Mathematics  
 Session IX: Chris Henley Memorial

Session X, XI: Surface and Overlayers  
 Session XII: Dynamics  
 Session XIII: Future directions of QC research  
 Session XIV: Composites & Applications  
 KU: Kathmandu University  
 TU: Tribhuvan University  
 DLR: Dhulikhel Lodge Resort

# Detailed Program

## 18th Sunday

<b>Tutorial (chair: J Ledieu)</b>			
09:20			Registration open at Dhulikhel Lodge Resort
11:40	12:40	Smerdon	Fibonacci, Penrose, Harry Potter: an introduction to the strange world of quasicrystals
12:40	13:40	Gomez	Structure analysis of icosahedral quasicrystals and approximants by X-ray diffraction
13:40	14:10	Refreshment	
14:10	15:10	Sato	Physics hidden in open space between heavy fermions and quasicrystals
16:00		Opening ceremony	
18:15		Welcome dinner	

## 19th Monday

<b>Session I: Formation, Growth, Soft Matter Quasicrystals (chair: C Gomez)</b>			
09:15	09:20		Opening remarks
09:20	09:50	Dotera	Bronze-mean hexagonal quasicrystal ( <b>invited</b> )
09:50	10:10	Ishimasa	Dodecagonal quasicrystal in Mn-based alloy
10:10	10:30	Boulet	Two types of QC approximant in the Ce-Au-Ge system
10:30	10:50	Shahi	Synthesis characterizations and hydrogenation behavior of as quenched $Ti_{45+X}Zr_{38-X}Ni_{17}$ ( $x=3, 5, 8$ ) nano quasicrystalline ribbons
10:50	11:20	Coffee	
<b>Session II: Structure and Modeling (chair: H Takakura)</b>			
11:20	11:40	YamadaT	Atomic structures of ternary Yb-Cd-Mg icosahedral quasicrystals
11:40	12:00	SinghA	Deformation of icosahedral quasicrystal in a composite of Mg-Zn-Y alloy during severe plastic deformation
12:00	12:20	Dong	Quasicrystal composition formulas and the hardness evaluation via the cluster-plus-glue-atom model
12:20	12:40	Buganski	The statistical description of the Cd-Yb icosahedral quasicrystal with the application of the novel concept of the phason disorder correction
12:40	13:10	Jana	Structure and stability of $AuZn_{2.1}$ – a $\gamma$ -brass related complex phase in the Au-Zn system ( <b>invited</b> )
13:10	14:20	Lunch	
<b>Session III: Structure and Modeling (chair: W Steurer )</b>			
14:20	14:50	Abe	Ultrahigh-resolution STEM combined with multivariate analysis for decagonal quasicrystals ( <b>invited</b> )
14:50	15:10	Wolny	Fundamentals of statistical description of diffraction pattern of crystals

15:10	15:30	Sugiyama	Middle range ordering realized in Zr-Pt amorphous alloy and quasicrystalline approximants
15:30	15:50	Chodyn	Generalized Penrose tiling as a model for structure refinement of decagonal quasicrystals
15:50	16:20	Coffee	
<b>Session IV: Electronic Properties (chair: JM Dubois )</b>			
16:20	16:40	Edagawa	Critical photonic states in 2D photonic quasicrystals
16:40	17:00	Kee	Ultraflattened Dispersion Properties of Photonic Quasicrystal Fibers
17:00	17:20	Lifshitz	Fibonacci Bloch functions
17:20	17:40	Subramanian	Weakly nonlinear analysis of three-dimensional quasicrystals using Homotopy continuation
17:40	18:00	Break	
18:00	20:00	Poster session with dinner	
20:00	21:00	Cultural program	

## 20th Tuesday

<b>Session V: Electronic and Transport Properties (chair: J Dolinsek )</b>			
09:20	09:50	Widmer	Fermi states and anisotropy of Brillouin zone scattering in the decagonal Al–Ni–Co quasicrystal ( <b>invited</b> )
09:50	10:10	Kitahara	Unified cluster-based description of valence Bands in AlIr, RuAl <sub>2</sub> , RuGa <sub>3</sub> , and Al–TM quasicrystalline approximants
10:10	10:30	Koga	Valence fluctuations in heavy fermion system on the Penrose lattice: real-space dynamical mean-field approach
10:30	10:50	Kimura	Search for semiconducting quasicrystal and high-performance thermoelectric material
10:50	11:20	Coffee	
<b>Session VI: Electronic and Transport Properties (chair: R Lifshitz)</b>			
11:20	11:40	Dolinsek	Schottky effect in rare-earth-containing quasicrystals
11:40	12:00	Laissardiere	Anomalous quantum diffusion in quasicrystals and approximants
12:00	12:20	Nicolas Macé	Gap structure and topological indices on the Fibonacci quasicrystal
12:20	12:40	Deguchi	Magnetism and superconductivity in Icosahedral quasicrystals and approximants with Tsai-type clusters
12:40	13:00	Elena	Magnetic charges in quasiperiodic vertex models
13:00	14:20	Lunch	
<b>Session VII: Magnetic Properties (chair: R Tamura)</b>			
14:20	14:50	Takemori	Local and short-range electron correlation effects on the Penrose lattice ( <b>invited</b> )

14:50	15:10	Sugimoto	Phenomenological magnetic model in Tsai-Type approximants
15:10	15:30	Kreyssig	Magnetic order in RCd6 single crystals – the approximants to the spin-glass i-R-Cd quasicrystals
15:30	15:50	Hiroto	Neutron-scattering study on the quasicrystal approximants Au-Si-R (R = rare-earths)
15:50	16:20	Coffee	
		<b>Session VIII:</b>	<b>Magnetic Properties/Mathematics (chair: A Goldman)</b>
16:20	16:50	Jagannathan	Screening of magnetic impurities in quasicrystals ( <b>invited</b> )
16:50	17:10	Tamura	Magnetic properties of Au-based Tsai-type approximants
17:10	17:30	Gullo	Equivalence classes of Fibonacci lattices and their similarity properties
17:30	17:50	Fang	Fractality in quasicrystals and prime number distribution
17:50	18:00	Break	
18:00	20:00	Poster session with dinner	
20:00	21:00	Cultural program	

### 21st Wednesday

		<b>Session IX:</b>	<b>Chris Henley Memorial Session (chair: M Widom)</b>
08:40	09:00	Mihalkovic	Finite temperature structure and stability of i-AlCuFe and i-AlMnPd from realistic simulations
09:00	09:20	Fujita	Canonical-cell icosahedral quasicrystals?
09:20	09:50	Ben-Abraham	Brick tiling ( <b>invited</b> )
09:50	10:10	Boyle	Coxeter pairs, Ammann patterns and Penrose-like tilings
10:10	10:30	Ajlouni	An ancient rule for constructing dodecagonal quasi-periodic formations
10:30	Move to Tribhuvan University (tea/coffee in bus)		
		<b>Public Lecture by Dan Shechtman at Tribhuvan University (chair: NP Adhikari)</b>	
12:00	13:00	Shechtman	<b>Technological Entrepreneurship - Key to World Peace and Prosperity</b>
13:00	22:00	Lunch followed by excursion and conference dinner	

### 22nd Thursday

		<b>Session X:</b>	<b>Surface and Overlayers (chair: R McGrath)</b>
09:20	09:50	Gaudry	First surface structure determination of a quasicrystalline approximant using combined surface x-ray diffraction and ab initio calculations ( <b>invited</b> )

09:50	10:10	Ledieu	Structural investigation of the Al <sub>13</sub> Ru <sub>4</sub> (010) surface
10:10	10:30	Fournee	Self-assembling of 5-fold symmetric molecules on quasicrystalline surfaces
10:30	10:50	Coates	Growth of modules on complex Al-based intermetallic compounds: role of order of surface structural complexity
10:50	11:20	Coffee	
		<b>Session XI:</b>	<b>Surface and Overlayers (chair: E Gaudry)</b>
11:20	11:40	Pussi	Coverage-dependent structural phase transformations in the adsorption of pentacene on an aperiodically modulated Cu film by DFT
11:40	12:00	Foerster	Growth and decay of oxide quasicrystals
12:00	12:20	Widdra	Structural analysis of approximants for the BaTiO <sub>3</sub> -derived oxide quasicrystal
12:20	12:40	Yuhara	Compositional analysis of oxide quasicrystal : Ba-Ti-O film on Pt(111)
12:40	13:00	Dubois	A complex Self-lubricating, low-friction, wear-resistant Al-based quasicrystalline coatings
13:00	14:10	Lunch	
		<b>Session XII:</b>	<b>Dynamics (chair: K. Edagawa)</b>
14:10	14:30	Trebin	Phason dynamics in decagonal quasicrystals
14:30	14:50	Grimm	Diffraction of a simple non-Pisot inflation chain
14:50	15:10	Lory	Impact of complexity and atomic disorder on lattice dynamics and thermal properties in the complex metallic alloys o-Al <sub>13</sub> Co <sub>4</sub>
15:10	15:30	Liu	Diffuse scattering, phason fluctuations and atomic scale simulation in the Zn-Sc icosahedral quasicrystal
15:30	15:50	Strzalka	Diffraction pattern of quasicrystals with phononic and phasonic disorder – state of art
15:50	16:20	Coffee	
		<b>Session XIII:</b>	<b>Future Directions of Quasicrystal Research (chair: M de Boissieu )</b>
16:20	16:45	Steurer	Quasicrystal structure and growth models - a discussion of the status quo and of the still open questions ( <b>invited</b> )
16:45	16:55	Floor Discussion	
16:55	17:20	Goldman	Physical properties of quasicrystals ( <b>invited</b> )
17:20	17:30	Floor Discussion	
17:30	17:55	Julien	Current questions in mathematical quasicrystals (and beyond) ( <b>invited</b> )
17:55	18:05	Floor Discussion	
18:05	18:15	Break	
18:15	20:00	Poster session with dinner	
20:00	21:00	Cultural program	

**23rd Friday**

		<b>Session XIV:</b>	<b>Composites &amp; Applications (chair: C Dong)</b>
09:20	09:50	Pérez	Phase transitions toward complex electronic states and superperiodic structures in monophosphate tungsten bronzes ( <b>invited</b> )
09:50	10:10	Cini	Bioactivity of quasicrystalline-reinforced composite materials for 3D printing of medical implants
10:10	10:30	Leu	The microstructure and hydrophobic behavior of Al-Cu-Fe coating by plasma spraying
10:30	10:50	Yadav	Mechanical properties of carbon nano-variant reinforced quasicrystal composite
10:50	11:20	Coffee	
11:20	11:40	Chen	Characteristic smearing wear behavior of quasicrystals as abrasive materials
11:40	12:00	Dahal	American physical society publications and peer review process (Associate Editor, Physical Review B)
12:00	12:20	Conclusion	
12:20		Lunch and End of Conference	



# **Abstracts For Oral Presentations**

## **Fibonacci, Penrose, Harry Potter: an introduction to the strange world of quasicrystals**

Joe Smerdon

*Jeremiah Horrocks Institute, University of Central Lancashire, Preston PR1 2HE, United Kingdom*

When order is found in the physical world, it is practically always periodic and arises from the local interactions possible between identical units. This is the ordering in crystals, which are simple systems. When order is found in the living world - in complex systems - it is rarely periodic. Instead it shows up as spirals in the patterns of seeds on a sunflower, or in the segmented skin of a pineapple, or in the shell of a snail. Upon examining such apparently complex systems, it is often the case that there are very strong principles that are obeyed. The numbers of seeds in spirals in opposite directions are Fibonacci numbers, described by Fibonacci in the middle ages. The spiral in the shell of a snail follows the golden ratio, described by Euclid in 300 BC. The golden ratio and the Fibonacci sequence are inherent features of pentagonal ordering, described in its simplest form by Penrose in 1974. In 1982, Dan Shechtman discovered quasicrystals, which show all of these features in a previously unsuspected arena: the ordering of atoms in condensed matter, commonly called crystalline ordering. Not only was this development unsuspected, it was fought with such enthusiasm that it took 2 years to publish [1], after nearly destroying Shechtman's career.

Now we accept the existence of quasicrystals. Dan Shechtman received the Nobel prize in Chemistry in 2011. We are using them in diverse applications, from non-stick coatings for frying pans to lightweight parts for high-performance cars [2]. We also use the principles we learn by studying the ordering of these materials in some less obvious ways. The propagation of waves is affected by their interaction with lattices, leading to our understanding of the interactions of electrons within matter and their existence within Brillouin zones. The Brillouin zones of a quasicrystal, due to the higher orders of rotational symmetry, can be nearly spherical, which suggests interesting possibilities for the confinement and propagation of waves of whichever length scale we choose to build the quasicrystal upon. This has led to some recent developments in metamaterial lenses with negative refractive indices [3] and even a version of Harry Potter's invisibility cloak [4].

[1] Shechtman et al., Phys. Rev. Lett. 53 1951, 1984

[2] Kenzari et al., Sci. Technol. Adv. Mater. 15 024802, 2014

[3] Feng et al., Phys. Rev. Lett. 94, 247402, 2005

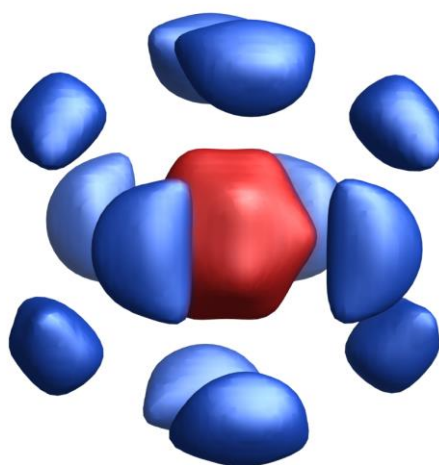
[4] Boriskina, Nature Photonics 9, 422–424, 2015

## Structure analysis of icosahedral quasicrystals and approximants by X-ray diffraction

Cesar Pay Gomez

*Department of Chemistry – Ångström Laboratory, Uppsala University, 751 21 Uppsala, Sweden*

In this tutorial lecture we will give an introduction to the various aspects and procedures involved in structure analysis of complex metallic alloys such as quasicrystals, approximants and other related phases. Special attention will be given to pitfalls related to positional and chemical order/disorder phenomena along with useful tips on how to avoid them. The examples will be based on binary and ternary phases related to the icosahedral Yb-Cd quasicrystal.<sup>[1-3]</sup>



*Figure 1: Electron density at the cluster center of a ternary Tsai-type approximant showing a disordered tetrahedron (blue) partially replaced by a central Rare Earth atom (red).*

- [1] Gómez, C. P.; Tsai, A. P., *Comptes Rendus Physique* **15**, 30 (2014).
- [2] Takakura, H.; *et al.*, *Nature Materials* **6**, 58 (2007).
- [3] Gómez, C. P.; Lidin, S., *Physical Review B* **68**, 024203 (2003).

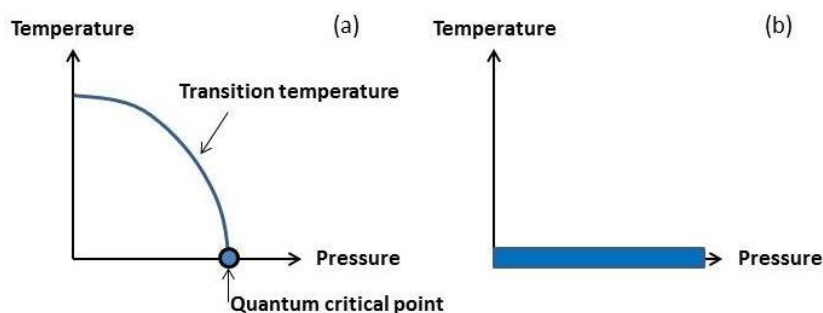
## Physics hidden in open space between heavy fermions and quasicrystals

Noriaki K. Sato

*Department of Physics, Graduate School of Science,  
Nagoya University, Nagoya 464-8602, Japan*

Heavy fermions are materials in which  $f$ -electrons travel over the crystal lattice while feeling strong Coulomb interaction among them. Due to this repulsive interaction, the  $f$ -electrons become less mobile than free electrons (that are usually  $s$ ,  $p$ , and  $d$ -electrons), resulting in the introduction of heavy mass into the  $f$ -electrons. In the heavy fermions, the effective mass of charge carriers can be thousands of times greater than that in conventional metals like copper. One may think that the repulsive interaction among the electrons would prevent the heavy fermions from forming Cooper pairs that are needed to become a superconductor. Interestingly, some heavy fermions do show superconductivity at a very low temperature. This means that our understanding of physics is not enough to perfectly understand the physical properties in the metallic materials.

According to intensive studies on the heavy fermions, not only the superconductivity but also the unusual properties (called “non-Fermi liquid”) were found to emerge near a quantum critical point, where a phase transition occurs at zero temperature ( $T=0$ ) as shown in Fig.1(a); see, for example, ref. [1]. This quantum critical point is a singular point in the phase diagram, which may resemble a “black hole” in the space. Recently, novel kind of quantum critical phenomenon was discovered in a quasicrystal [2]; as shown in Fig.1(b), non-Fermi liquid was observed along a line, instead of a point. Here, quasicrystal is a metallic alloy possessing a nonperiodic yet long-range-ordered (quasiperiodic) arrangement of the atomic structure. This unexpected observation opened a door to new physics that is expected to be hidden in the interdisciplinary field between the heavy fermions and the quasicrystals. In my lecture, you will be invited to this new world.



*Fig.1. Temperature vs Pressure phase diagram. Conventional case (a) and unconventional case of quasicrystal (b).*

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## Bronze-mean hexagonal quasicrystal

Tomonari Dotera<sup>1</sup>, Shinichi Bekku<sup>1</sup>, and Primož Ziherl<sup>2,3</sup>

<sup>1</sup>*Department of Physics, Kindai University, 3-4-1 Kowakae, Higashi-Osaka 577-8502, Japan*

<sup>2</sup>*Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia*

<sup>3</sup>*Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia*

Quasicrystals are believed to have nontraditional crystallographic symmetry such as decagonal, dodecagonal, and octagonal rotational symmetries. Indeed, quasiperiodicity is characterized by two or more spacings whose length ratio is an irrational number associated with the unconventional rotational symmetry: the golden mean Penrose tiling with decagonal symmetry, the silver mean Ammann-Beenker tiling with octagonal symmetry, and the the platinum mean Stampfli tiling with dodecagonal symmetry. Contrary to the accepted wisdom that quasicrystals are originated from the unusual rotational symmetries, we present a “6-fold” quasiperiodic tiling related to the bronze mean, which number has been missing in the literature. Using a two-lengthscale potential, which has turned out to be a minimal and efficient tool to produce quasicrystals [1], we have performed simulations of a particle system and obtained a random-tiling of the 6-fold quasicrystal. Since the novel tiling is akin to the 12-fold square-triangle quasiperiodic tiling, it is expected to realize in soft and other materials [2]. Moreover, by varying the geometry of the pattern we generate a continuous sequence of structures, which provide an alternative interpretation of quasicrystalline approximants observed in several metal-silicon alloys. Thus the new tiling relates to both materials science and the mathematical basis of quasicrystals [3].

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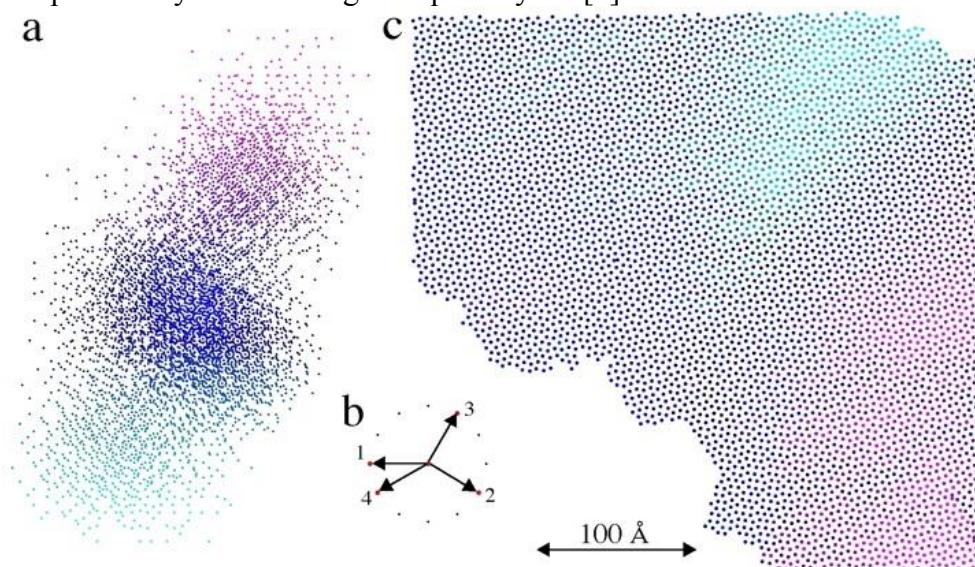
## Dodecagonal quasicrystal in Mn-based alloy

Tsutomu Ishimasa

*Graduate School of Engineering, Hokkaido University, Sapporo, Hokkaido 060-8628, Japan*

The dodecagonal quasicrystal, which shows 12-fold diffraction symmetry, has been discovered recently in the Mn-based quaternary alloy containing Cr, Ni and Si [1]. The purpose of this study is to clarify structural properties of the quasicrystal with the help of spherical aberration (Cs) corrected electron microscopy.

The structural analysis was carried out in the framework of the projection method by indexing directly the electron microscope images observed along the 12-fold axis. This analysis has revealed non-periodic tiling in relatively wide area ( $350 \text{ \AA} \times 350 \text{ \AA}$ ), in which an equilateral triangle and a square are arranged as presented in Fig. 1c. The common edge length of the tiles is  $4.6 \text{ \AA}$ . Remarkable feature of the tiling in the phason space is the limited number of domains, each of which has different center (Fig. 1a). Correspondingly, three domains are clearly observed in the physical space, which are indicated by blue, green or purple in Fig. 1c. It is concluded that the present state consists mainly of such small quasicrystal domains of  $100 \text{ \AA}$ -scale. This is the first experimental indication of the presence of an acceptance domain, and thus quasiperiodicity in a dodecagonal quasicrystal [2].



*Figure 1: Triangle-square tiling (c) and its corresponding distribution (a) in the phason space. (b) Four basis vectors of the phason space as the size reference.*

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## Two types of QC approximant in the Ce-Au-Ge system

P. Boulet<sup>1</sup>, M.C. de Weerd<sup>1</sup>, O. Tougait<sup>2</sup>, J. Ledieu<sup>1</sup> and V. Fournée<sup>1</sup>

<sup>1</sup>*Institut Jean Lamour, UMR 7198 CNRS- Université de Lorraine, Nancy, France*

<sup>2</sup>*Unité de Catalyse et de Chimie du Solide, UMR 8181 CNRS, Université de Lille 1, France*

Since the discovery of the stable binary Cd<sub>5.7</sub>Yb [1] and Cd<sub>5.7</sub>Ca [2] icosahedral quasicrystals, there has been an increasing interest in these quasicrystalline structures and their approximants. These quasicrystalline phases, known as Tsai-type QCs, and their related approximants (Cd<sub>6</sub>Yb Type, SG: Im-3) are made of concentric shells of disordered tetrahedra, dodecahedra, icosahedra, icosidodecahedra and defected triacontahedra from the inside out.

Similar approximant structures, crystallizing with the body centered space group Im-3, have been reported in ternary systems RE-Au-X with X= Sn [3-5] and with RE = Ce, Pr, Nd, Sm, Eu, Gd, Dy and Tb. This type of structure was also reported to exist with X= Al [6,7], Si and Ge and with RE = Gd [8], Tb [9] and Yb [8]. All these phases crystallize within a non-negligible homogeneity range. Depending on their exact stoichiometry, there are differences in the occupancy of some specific crystallographic sites, especially those around the tetrahedron located at the center of the Tsai-type cluster.

In this frame, we have investigated the Ce-Au-Ge phases around the Ce<sub>3</sub>Au<sub>13</sub>Ge<sub>4</sub> quasicrystalline composition using the Czochralski growth method. While the composition is identical across the ingot from EDX analyses, two different structures have been identified by XRD powder measurements. A single crystal XRD analysis performed on the batch of the material reveals a body centered cubic structure (Im-3) isotypic to those previously reported for the Sn-containing systems [3] with  $a = 14.857 \text{ \AA}$ . A similar analysis carried out on a specimen collected in the region corresponding to the beginning of the Czochralski pulling indicates the presence of a second structure. The latter is indexed as a cubic face centered unit cell with  $a = 21.153 \text{ \AA}$ , i.e. almost  $2^{1/2}$  time the lattice parameter of the body centered crystal structure. Single crystal XRD studies confirm such unit cell with the non-centrosymmetric space group F-43m, pointing out the strong relationship of this structure with the  $\gamma$ -brass structure type.

In this paper, these two crystal structures will be presented with their relationship.

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19<sup>th</sup> September, Monday

## **Synthesis characterizations and hydrogenation behavior of as quenched $\text{Ti}_{45+x}\text{Zr}_{38-x}\text{Ni}_{17}$ (x=3, 5, 8) nano quasicrystalline ribbons**

Rohit R Shahi<sup>1</sup>, T.P. Yadav<sup>2</sup>, M.A. Shaz<sup>2</sup>, O.N. Srivastava<sup>2</sup>

<sup>1</sup>*Department of Physics Motilal Nehru National Institute of Technology Allahabad-211004  
India*

<sup>2</sup>*Department of Physics, Banaras Hindu University, Varanasi-221005, India*

The present study describes the synthesis characterization and hydrogen storage behavior of  $\text{Ti}_{45+x}\text{Zr}_{38-x}\text{Ni}_{17}$  (x=3,5,8) nano quasicrystalline ribbons synthesized through rapid solidification technique. The nano quasicrystalline ribbons of alloys are synthesized at Cu-wheel speed of 45 m/sec. Moreover, the investigations further describe the effect of various compositions of Ti and Zr on the structure, microstructure of synthesized ribbons and their correlation with hydrogen storage characteristics of as quenched nanoquasicrystalline ribbons. It is found that the hydrogen storage capacity of these ribbons increases with increasing the content of Ti. The micro structural correlation with hydrogen storage performance of these alloys will be discussed and described in details in the presentation.



## Atomic structures of ternary Yb-Cd-Mg icosahedral quasicrystals

Tsunetomo Yamada<sup>1</sup>, Hiroyuki Takakura<sup>2</sup>, An Pang Tsai<sup>1</sup>

<sup>1</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577 Japan*

<sup>2</sup>*Division of Applied Physics, Faculty of Engineering, Hokkaido University, Sapporo, 060-8628, Japan*

Discovery of the binary icosahedral (i) quasicrystal (QC) YbCd<sub>5.7</sub> led to a breakthrough in the field of QCs by allowing a detailed analysis of its atomic structure [1, 2]. On the other hand, structure determination for ternary or multinary QCs remains a challenging problem since a substitutional disorder must be taken into account in addition to positional disorder. To address these problems inherent in the samples, we focus on the i-Yb-Cd-Mg QC by the following reasons. Firstly, it has large solid solubility of Mg into Cd up to about 60 % [3], hence, the relative occupancies of Cd and Mg can be examined along with Mg contents. Secondly, it is thought to be isostructural to the i-YbCd<sub>5.7</sub> and thus the structure refinement is possible based on the i-YbCd<sub>5.7</sub> model.

We prepared single-grained crystals of i-Yb-Cd-Mg with different Mg contents up to 46.4 at.%. Diffraction experiments were carried out using an in-house X-ray diffraction system (Mo target) and 1476 common unique reflections for five samples were measured in the resolution limit equal to 0.8 Å<sup>-1</sup>. Analysis of six-dimensional (6-D) electron densities, obtained by applying the low-density elimination method [4], revealed that a systematic decrease of the electron densities at the vertices of a primitive 6-D lattice. This demonstrates that Mg preferentially occupies the vertices sites, which is fully consistent with a previous report [5]. Structure refinements based on the i-YbCd<sub>5.7</sub> model were carried out for two samples with different Mg contents, Yb<sub>15.5</sub>Cd<sub>68.4</sub>Mg<sub>16.1</sub> and Yb<sub>15.0</sub>Cd<sub>38.5</sub>Mg<sub>46.4</sub>. The details of resulting atomic structures and refined relative occupancies of Cd and Mg in terms of the shell structure of Tsai-type cluster will be presented.

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## **Deformation of icosahedral quasicrystal in a composite of Mg-Zn-Y alloy during severe plastic deformation**

Alok Singh, Dudekula Althaf Basha, Hidetoshi Somekawa and Koichi Tsuchiya

*Research Center for Structural Materials, National Institute for Materials Science,  
1-2-1 Sengen, Tsukuba 305-0047, Ibaraki, Japan*

It has been shown recently that very high strengths can be achieved in magnesium alloys reinforced with icosahedral (i-) phase in Mg-Zn-Y alloys [1-2]. Development of such light weight alloys is very important for producing more environment friendly automobiles which consume less fuel. In this work we have studied the deformation behavior of the i-phase under severe plastic deformation in a Mg-12Zn-2Y (at%) alloy.

The Mg-12Zn-2Y (at%) alloy was prepared by melting high purity elements in an electric furnace and cast into a cylindrical steel mold. The casting was annealed at 400° C for 10h followed by furnace cooling. Disc samples of 10 mm diameter and 0.85 mm thickness were machined from the alloy and subjected to severe plastic deformation (SPD) by high pressure torsion (HPT), for various number of turns N. Microstructure of the samples was studied by X-ray diffraction and transmission electron microscopy (TEM).

The i-phase formed as eutectic phase in the interdendritic spaces of  $\alpha$ -Mg phase with arm widths in the range of 10 to 20  $\mu\text{m}$ . Due to HPT strain, severe deformation occurred in the Mg-matrix, as described in our earlier study on a Mg-3Zn-0.5Y alloy [3]. Recrystallization of  $\alpha$ -Mg grains occurred over i-phase. No noticeable deformation was noticed in the i-phase until an applied strain of  $N=3$ . Formation of planar low angle boundaries was observed on fivefold planes. Structure of dislocations and low angle boundaries have been studied to determine the deformation behavior of the i-phase. Interaction of the Mg matrix dislocations with the i-phase has also been of prime interest in this study.

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19<sup>th</sup> September, Monday

## **Quasicrystal composition formulas and the hardness evaluation via the cluster-plus-glue-atom model**

Chuang Dong

*Key Lab of Materials Modification by Laser, Ion, and Electron Beams (Ministry of Education), School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, China*

Composition rule and hardness of Al-based binary metastable and ternary stable quasicrystals are explored using the cluster-plus-glue-atom model and the valence electron concentration factor. Compositions of binary Al-TM (TM=Cr to Ni) quasicrystals are interpreted with a unified cluster formula [icosahedron](glue)<sub>0 or 1</sub>. Icosahedral quasicrystals are expressed by an icosahedron plus zero glue atom [icosahedron](glue)<sub>0</sub>, characterized by  $e/a \sim 1.83 - 1.85$ , while decagonal quasicrystals are expressed by an icosahedron plus one glue atom, with  $e/a \sim 1.71 - 1.78$ . The total electrons accommodated in unit cluster formulas of different Al-TM quasicrystals have the same value, approaching 24, which implies that the cluster formulas are both chemical and electronic structural units. A quantitative description of the structure-property relationships of quasicrystals was also given. It was shown within the framework of this model that the hardness of quasicrystals are determined by the number of the ruptured weakest bonds per unit cluster formula. Typically, theoretical hardness values of 8~9 GPa was obtained using ~18 broken inter-cluster bonds, which accounts for half of all the inter-cluster bonds. The unit cluster formulas would act as rigid units during deformation and cracking.

Key words: Quasicrystals; Cluster-plus-glue-atom model; Hardness

19<sup>th</sup> September, Monday

## **The statistical description of the Cd-Yb icosahedral quasicrystal with the application of the novel concept of the phason disorder correction**

Ireneusz Buganski<sup>1</sup>, Radoslaw Strzalka<sup>1</sup>, Hiroyuki Takakura<sup>2</sup>, Janusz Wolny<sup>1</sup>

<sup>1</sup>*AGH – University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland*

<sup>2</sup>*Division of Applied Physics, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido, 060-8628, Japan*

Up to now the correction of the diffraction peaks' intensities with respect to phasons is made by application of the generalized Debye –Waller formula (D-W) [1]. Due to recent discovery showing such formula can lead to characteristic bias of the calculated intensities [2] we decided to obtain a new kind of additive correction instead of multiplicative D-W. The correction which takes into account phason flips in random places of aperiodic tiling was obtained for Ammann tiling and can be incorporated to the formula of the structure factor. Within this model the probability of flip occurrence is the parameter of fitting which gives clear physical interpretation. Derived formula was applied to investigate structure of Cd<sub>5.7</sub>Yb icosahedral quasicrystal and check if the quality of refinement procedure will result with better convergence of the proposed model with experimental data in comparison to the cluster model with the usage of D-W formula [3].

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## Structure and stability of AuZn<sub>2.1</sub> – a $\gamma$ -brass related complex phase in the Au-Zn System

Partha Pratim Jana<sup>1,2</sup>, S. Thimmaiah<sup>3</sup>, S. Lidin<sup>2</sup>, G. J. Miller<sup>3</sup>

<sup>1,2</sup> Department of Chemistry, Indian Institute of Technology Kharagpur, India-721302

<sup>2</sup> Department of Chemistry, Lund University, 22100 Lund, Sweden

<sup>3</sup> Department of Chemistry, Iowa State University, and Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, United States

$\gamma$ 1-AuZn<sub>2.1</sub> in the Au-Zn binary system has been synthesized via zinc self flux method and the structure has been analyzed by single crystal X-ray diffraction. The compound AuZn<sub>2.1</sub> crystallizes in the trigonal space group  $P31m$  (157) and unit cell contains ~ 227 atoms. The compound AuZn<sub>2.1</sub> is a  $\sqrt{3}a \times \sqrt{3}b \times c$  -superstructure of a rhombohedrally distorted  $\gamma$ -Au<sub>5-x</sub>Zn<sub>8+y</sub> phase<sup>1</sup>. The structure is mostly tetrahedrally closed packed (Figure 1). The compound is found at a valence electron concentration value of 1.68 e/a. The formation of the compound can be understood within the framework of the Hume-Rothery stabilization mechanism<sup>2</sup>.

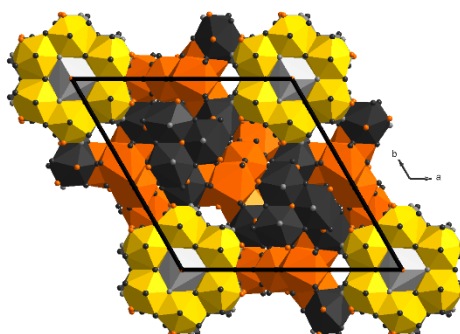


Figure 1. Polyhedral representation of the structure of  $\gamma$ 1-AuZn<sub>2.1</sub> along [0 0 1].

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## Ultrahigh-resolution STEM combined with multivariate analysis for decagonal quasicrystals

T. Seki, M. Ohura and E. Abe

*Department of Materials Science & Engineering, University of Tokyo, 113-8656, Japan*

For the last decade, the atomic-resolution scanning transmission electron microscopy (STEM) has provided remarkable progresses in determining decagonal quasicrystal (d-QC) structures [1], particularly by unveiling the local cluster symmetry as well as the relevant atomic configurations through the element-sensitive Z-contrast imaging. Recent ultrahigh-resolution imaging with aberration-corrected STEM has provided further insights of local cluster symmetry; atomic configurations within the cluster are not strictly identical but slightly different due to phason-related disorder even in the best-ordered d-QCs specimen, breaking weakly the underlying ideal symmetry for each of the local clusters [2]. During the x-ray diffraction analysis, such weak disorder may be averaged over the entire specimen, and hence the true symmetry of the cluster may possibly be misled without preliminary knowledge about cluster symmetry.

In the present paper, we have attempted to determine the structure of several d-QCs at the highest reliability, based on a combination between ultrahigh-resolution STEM and hyperspace x-ray crystallography [3]. Through a multivariate analysis of the STEM images [2], we first determine the fundamental cluster and evaluate the relevant local degree of order. Then, the cluster model is compared with x-ray analysis results, during which the model convergence is judged based on not the R-factor alone but comprehensive evaluations, including direct comparison of the Fourier map with the relevant STEM images. We will discuss how we should judge/approach the true solution of complex quasicrystal structures.

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## Fundamentals of statistical description of diffraction patterns of crystals

Janusz Wolny<sup>1</sup>, Ireneusz Buganski<sup>1</sup> and Radoslaw Strzalka<sup>1</sup>

<sup>1</sup>*Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland*

The statistical method applied to diffraction analysis is now a complete theory which deals equally well with periodic and non-periodic crystals, including quasicrystals. In this presentation we show the fundamentals of statistical description applied to aperiodic crystals in various aspects. Basic concept of a method is the average unit cell which is a statistical probability distribution  $P$  of atomic positions with respect to some reference lattices [1]. Those lattices are calculated with lattice parameters related to the basic scattering vector  $k_0$ . The distribution is a powerful tool which allows to calculate structure factor of any type of structure. The shape of envelope function that connects all diffraction maxima can be derived as simple Fourier transform of a distribution function. Moreover, distributions are sensitive to any disorder introduced to ideal structure – phonons and phasons. The latter are particularly important in case of quasicrystals, however the consistent theory of phasonic disorder is still not available [2]. The statistical method deals very well with phason flips and may be used to redefine phasonic Debye-Waller correction factor in a new approach [3].

In our presentation we particularly focus on application of the statistical approach to the peak's profile interpretation. We show how the relation between distributions calculated for basic scattering vector  $k_0$  and its integer multiple  $nk_0$ , respectively  $P(k_0)$  and  $P(nk_0)$ , determine the shape of a diffraction maximum. It will be shown that the average unit cell can be equally well applied to a description of Bragg peaks as well as other components of diffraction pattern, namely continuous and singular continuous components.

Calculations performed within statistical method are equivalent to the ones from multidimensional analysis, currently most commonly used in structure modeling of quasicrystals. The atomic surface, also called occupation domain, which is the basic concept behind multidimensional models, acquires more physical interpretation if compared to average unit cell [4].

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19<sup>th</sup> September, Monday

## Middle range ordering realized in Zr-Pt amorphous alloy and quasicrystalline approximants

Kazumasa Sugiyama<sup>1</sup>, Toru Kawamata<sup>2</sup> and H.Arima<sup>1</sup>

<sup>1</sup>*Institute for Materials Research (IMR), Tohoku University,  
Sendai, Aoba-ku 980-8577 Japan*

<sup>2</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku  
University, Sendai Aoba-ku 980-8577 Japan*

The short to medium range atomic ordering in the amorphous alloys has been attracted many researcher's attention because the interesting material properties of amorphous alloys are closely associated with their atomic arrangement. Previous reports of Zr-Pt amorphous alloy have suggested the icosahedral-like local atomic arrangement together with the enhanced middle range ordering of the Pt-Pt correlation [1, 2]. However, the relationship between icosahedral topological short range ordering and middle range ordering, which contribute to enhancement of medium range Pt-Pt correlation, have not been elucidated yet.

The partial  $g_{ij}(r)$ s and  $S_{ij}(Q)$ s in Zr<sub>80</sub>Pt<sub>20</sub> amorphous alloy obtained by AXS-RMC analysis [3] suggest the enhancement of strong Zr-Pt bonding together the icosahedral-like coordination around Pt. This structural feature could not be realized in the common dense random packing (DRP) model, and is associated well with the behavior of Zr-Pt amorphous alloy, where an icosahedral phase can be crystallized by the appropriate heat treatment. Additionally, the pre-peak signal found in  $S_{PtPt}(Q)$  was also attributed to the Pt-Pt medium range correlation of about 0.4-0.5nm. The further discussion by using common neighbor analysis revealed that the medium range ordering of Pt-Pt pair was enhanced by the in homogeneity for chemical species and the corresponding geometrical packing fraction. These geometrical features found in Zr<sub>80</sub>Pt<sub>20</sub> amorphous alloy appears to be similar to those in Mackay clusters found in the crystalline approximants for the icosahedral phase. This paper demonstrates the results of our new approach by using Bernal polyhedral analysis (BPA) in order to discuss the geometrical similarity between Zr<sub>80</sub>Pt<sub>20</sub> amorphous alloy and icosahedral clusters.

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## Generalized Penrose tiling as a model for structure refinement of decagonal quasicrystals

M. Chodyń, P. Kuczera and J. Wolny

*Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland*

The Generalized Penrose Tiling (GPT)[1,2] can be considered a promising alternative for Penrose Tiling (PT) as a model for decagonal quasicrystal refinement procedure, particularly in the statistical approach (also called the Average Unit Cell (AUC) approach) [3]. The statistical method using PT has been successfully applied to structure optimization of various decagonal phases [4]. An application of the AUC concept to the GPT[5,6] will be presented. In the higher dimensional ( $nD$ ) approach, PT is obtained by projecting a 5D hypercubic lattice through a window consisting of four pentagons, called the atomic surfaces (ASs), in perpendicular space. The vertices of these pentagons together with two additional points form a rhombicosahedron. The GPT is created by projecting the 5D hypercubic lattice through a window consisting of five polygons, generated by shifting the ASs along the body diagonal of the rhombicosahedron. Three of the previously pentagonal ASs will become decagonal, one will remain pentagonal and one more pentagon will be created (for PT it is a single point). The structure of GPT will depend on the shift parameter. Its building units are still thick and thin rhombuses, but the matching rules and the tiling change. A diffraction pattern of GPT has peaks in the same positions as regular PT, however, their intensities are different.

First, to test possibility of refining of shift parameter, binary decagonal quasicrystal structure with arbitrary decoration for a given shift value was simulated. After successfully fitting the simulated tiling, the procedure was applied to the experimental diffraction data decagonal Al-Cu-Rh quasicrystal.

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## Critical photonic states in 2D photonic quasicrystals

Yuta Kawamata, Hiroyasu Fujikawa and Keiichi Edagawa

*Institute of Industrial Science, The University of Tokyo, Tokyo 153-8558 Japan*

Electronic states in quasicrystals have attracted considerable attention since the discovery of a quasicrystal by Shechtman et al. in 1984 [1]. Theoretical investigations have suggested that some electronic eigenstates in quasicrystals are critical, i.e., neither extended over the system nor localized exponentially [2]. However, the formation of such critical states in real quasicrystalline materials has not unambiguously been demonstrated.

Photonic crystals are artificial periodic structures of dielectrics with a period comparable to light wavelength. Many researches of them have recently been conducted because of their great potential for applications to light manipulation. In this work, we have investigated the photonic states in photonic quasicrystals, i.e., artificial quasicrystalline structures of dielectrics, focusing on whether critical photonic states are formed.

Photonic band structure calculations were done for a series of crystal approximants to a two-dimensional dodecagonal quasicrystal. Here, the structures consisted of the arrangement of dielectric columns, and the calculations were performed by a plane-wave expansion method for the TM-mode. We analyzed the system-size ( $L$ ) dependence of ‘participation’, i.e.,  $P = \left( \int |\mathbf{E}(\mathbf{r})|^2 d\mathbf{r} \right)^2 / \int |\mathbf{E}(\mathbf{r})|^4 d\mathbf{r}$  of the electrical fields of the eigenstates in three different frequency regions: the region far below the bandgap (Region 1), that just below it (Region 2), and that just above it (Region 3). In Region 1, we found  $P \propto L^\alpha$  with  $\alpha \approx 2.0$ , indicating that the states are extended. On the other hand, in Region 2 and 3, we obtain  $\alpha = 1.56$  and  $1.58$ , respectively. Here,  $\alpha$  values of  $0 < \alpha < 2.0$  are indicative of critical photonic states. Multifractality of the photonic eigenstates was also analyzed.

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## Ultraflattened Dispersion Properties of Photonic Quasicrystal Fibers

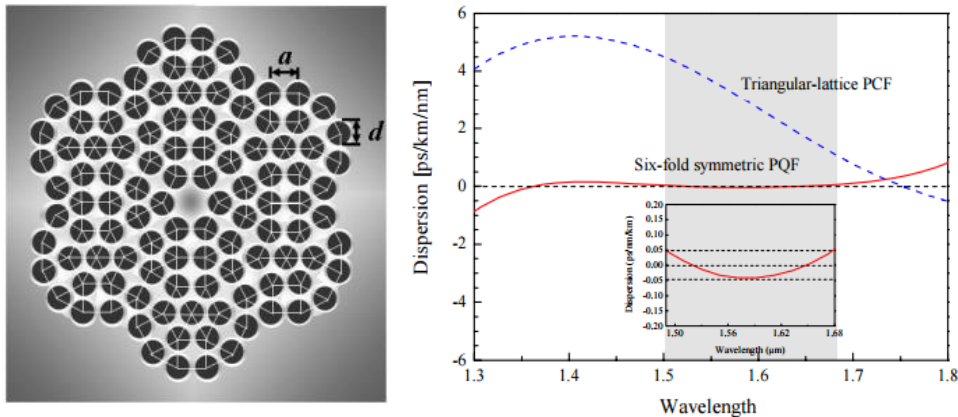
Soan Kim and Chul-Sik Kee

<sup>1</sup>*Advanced Photonics Research Institute, GIST, Gwangju 61002, South Korea*

Introducing quasiperiodic array of microscopic air holes in optical fibers could give rise to unique properties that were not found in the fibers having periodic array of air holes, photonic crystal fibers (PCFs). However, the properties of fibers with quasiperiodic arrays of air holes in cladding, photonic quasicrystal fibers (PQFs), have rarely been investigated.

In this talk, we investigated properties of the six-fold symmetric PQF and compared them with those of a triangular PCF having six-fold symmetry. The PQF exhibits larger cutoff ratio for endlessly single mode operation than that of a triangular PCF and almost zero ultraflattened chromatic dispersion ( $0 \pm 0.05 \text{ ps nm}^{-1} \text{ km}^{-1}$ ) in the wide wavelength range from 1.49 to 1.68  $\mu\text{m}$ . The nearly zero ultra-flattened dispersion property can be useful in the generation of flat and wideband supercontinuum and wavelength division multiplex communications systems.

Figure 1: (Right) Schematic cross section of a six-fold symmetric photonic quasicrystal fiber



and elementary units of the quasicrystal (dotted lines). (Left) Black circles denote air holes.  $a$  is the distance between neighboring air holes and  $d$  is the diameter of air holes. Dispersion of the six-fold symmetric PQF (red line) and a triangular lattice PCF (blue line) in the range from 1.3 to 1.8  $\mu\text{m}$  for  $d/a = 0.31$  and  $a = 2.41 \mu\text{m}$ . The gray region denotes the almost zero ultraflattened dispersion ( $0 \pm 0.05 \text{ ps nm}^{-1} \text{ km}^{-1}$ ) in the range from 1.49 to 1.68  $\mu\text{m}$ . The detailed dispersion behavior is shown in the inset.

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19<sup>th</sup> September, Monday

## Fibonacci Bloch Functions

Omri Lesser, Shahar Even-Dar Mandel, and Ron Lifshitz

*School of Physics & Astronomy, Tel Aviv University, Tel Aviv 69978, Israel*

It has been known for a long time that, in general, the Bloch theorem does not apply to quasicrystals [1]. Accordingly, single-electron eigenfunctions on typical models of quasicrystals exhibit algebraic decay, as opposed to the extended Bloch eigenfunctions that are observed in similar models of periodic crystals. Nevertheless, it is interesting to explore whether extended quasiperiodic Bloch functions may somehow emerge in realistic physical situations—either as superpositions of eigenfunctions, or even as true eigenfunctions of slightly modified quasiperiodic structures. If so, what is the nature of these quasiperiodic Bloch functions? How are they related to the structure of the underlying quasicrystalline potential? Are they characterized by the same kind of quantum numbers in reciprocal space as their periodic analogs? If so, is there an energy-momentum dispersion curve, or band structure, that is associated with these Bloch functions?

We study these questions using the familiar tight-binding model on the 1-dimensional Fibonacci quasicrystal. Indeed, we find that superpositions of relatively small numbers of nearly degenerate eigenfunctions give rise to extended quasiperiodic Bloch functions. These functions possess the structure of earlier ancestors of the underlying Fibonacci potential, and it is often possible to obtain different ancestors as different superpositions at the same energy. The quantum number that characterizes all of these ancestors is uniquely determined by the average energy of the superimposed eigenfunctions, giving rise to a very clear dispersion curve. We also find that Fibonacci-like Bloch functions emerge as eigenfunctions when a bit of static disorder is introduced into the otherwise perfect Fibonacci potential. These theoretical results may explain certain experimental observations [2,3].

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## Weakly Nonlinear Analysis of Three-Dimensional Quasicrystals using Homotopy Continuation

Priya Subramanian<sup>1</sup>, Andrew J. Archer<sup>2</sup>, Edgar Knobloch<sup>3</sup> and Alastair Rucklidge<sup>1</sup>

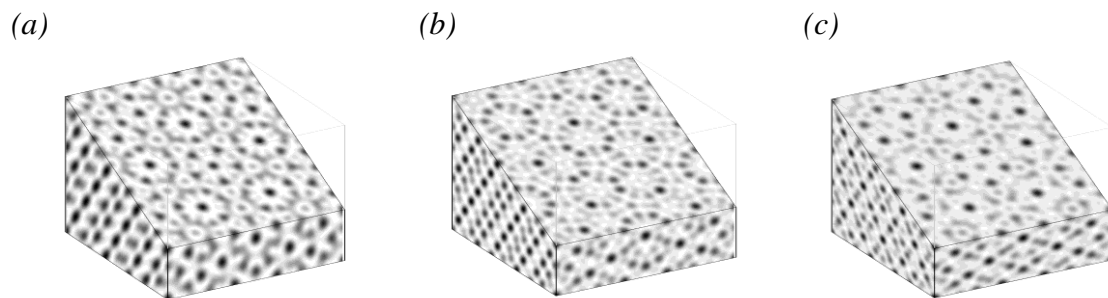
<sup>1</sup>*Department of Applied Mathematics, University of Leeds, Leeds, LS2 9JT, UK*

<sup>2</sup>*Department of Mathematical Sciences, Loughborough University,  
Loughborough LE11 3TU, UK*

<sup>3</sup>*Department of Physics, University of California at Berkeley, Berkeley CA 94720, USA*

The formation and stability of three-dimensional soft-matter quasicrystals (QCs) can be understood using a model system that employs a phase field crystal approach. Recent results using this approach indicate that the requirements for the presence of two-dimensional QCs, viz. periodic density modulations with two wavelengths (within a factor of two) and strong resonant nonlinear interactions, also suffice for the formation of three-dimensional icosahedral QCs [1].

Regular 5-fold icosahedral quasicrystals are obtained as the global minima of this model system in a parameter range where both interacting wavelengths are close to marginal stability. Simple structures such as lamellae, columnar hexagons and body-centered cubic crystals at each of the two length scales are the other possible global minimum energy structures. Weakly nonlinear approximations to the mode amplitudes corresponding to these and other more complicated patterns are obtained from appropriate amplitude equations. We employ the method of homotopy continuation to solve this coupled set of algebraic equations (computational algebraic geometry) and to determine all the small amplitude real solutions of these equations [2]. The availability of the full set of solutions makes it possible to calculate the global minima of the free energy among all pattern types and to identify new solutions corresponding to different symmetry subspaces of the icosahedral symmetry superset. We obtain axial quasicrystalline structures as shown in Figure 1(a-b) in addition to the simple regular structures such as lamellae, columnar rhombii, hexagons and the fully icosahedral quasicrystal shown in Figure 1(c).



*Figure 1: Axial quasicrystalline structures with periodic stacking of a 2D quasicrystal structures with (a) periodicity at the larger wavelength and (b) periodicity at the smaller wavelength. (c) Fully icosahedral quasicrystal.*

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## Fermi states and anisotropy of Brillouin zone scattering in the decagonal Al–Ni–Co quasicrystal

V.A. Rogalev<sup>1</sup>, R. Widmer<sup>2</sup>, O. Gröning<sup>2</sup>, J.H. Dil<sup>1,3</sup>, F. Bisti<sup>1</sup>, L.L. Lev<sup>1,4</sup>, T. Schmitt<sup>1</sup>, V.N. Strocov<sup>1</sup>

<sup>1</sup> Department for Synchrotron Radiation and Nanotechnology (SYN), Swiss Light Source, Paul Scherrer Institute, Villigen CH-5232, Switzerland

<sup>2</sup> Department of Advanced Materials and Surfaces, EMPA, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland

<sup>3</sup> Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

<sup>4</sup> National Research Center Kurchatov Institute, Akademika Kurchatova Square 1, 123182 Moscow, Russia

Much effort has been devoted to understand the influence of the quasiperiodic order on the remarkable physical properties of quasicrystals (QC) [1]. The valence band electronic structure near the Fermi energy  $E_F$  in such materials is of special interest since it has a direct relation to their unusual physical properties. However, the Fermi surface (FS) topology as well as the mechanism of QC structure stabilization are still under debate. In the case of decagonal QC it is possible to directly compare properties along the quasiperiodic with those of the periodic direction. Here, we report the first observation of the three-dimensional FS and valence band dispersions near  $E_F$  in decagonal Al<sub>70</sub>Ni<sub>20</sub>Co<sub>10</sub> (d-AlNiCo) QCs using soft X-ray angle-resolved photoemission spectroscopy [2]. We show that the FS, formed by dispersive Al s-states, has a multicomponent character due to a large contribution from high-order bands. Moreover, we discover that the magnitude of the gap at the FS related to the interaction with Brillouin zone boundary (Hume-Rothery gap) critically differs for the periodic and quasiperiodic directions.

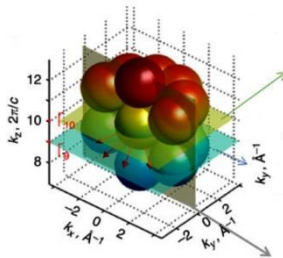


Figure 1: Sketch of the 3D FS observed in the current experiment with the planes corresponding to the different cuts at  $k_z=10(2\pi/c)$ ,  $k_z=9(2\pi/c)$  and  $k_y=0$ .

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20<sup>th</sup> September, Tuesday

## Unified cluster-based description of valence bands in AlIr, RuAl<sub>2</sub>, RuGa<sub>3</sub>, and Al–TM quasicrystalline approximants

Koichi Kitahara<sup>1</sup>, Yoshiki Takagiwa<sup>1,2</sup>, and Kaoru Kimura<sup>1</sup>

<sup>1</sup>*Department of Advanced Materials Science, The University of Tokyo, Kashiwa 277-8561, Japan*

<sup>2</sup>*National Institute for Materials Science, Tsukuba 305-0047, Japan*

Formation of pseudogap or narrow bandgap in some of group 13 element–transition metal (TM) intermetallic compounds including Al–TM quasicrystalline approximants had extensively been studied, and importance of hybridization between *sp*-orbitals of group 13 elements (or free electrons in a jellium) and *d*-orbitals of TM atoms were realized [1]. However the concept of *sp-d* hybridization cannot completely explain the formation of bandgap, especially the number of valence bands. For example, in the case of RuAl<sub>2</sub>, there are seven valence bands per ruthenium atom without considering spin degeneracy. While five out of the seven bands can be associated with *sp-d* bonding orbitals, the origin of the other two bands is unclear.

We studied the electronic band structures in AlIr, RuAl<sub>2</sub>, RuGa<sub>3</sub>, and Al–Cu–Ir quasicrystalline approximant [2] using maximally localized Wannier functions [3], which are representative orbitals corresponding to the bands in a specified energy range and can be constructed in principle without *a priori* assumption. In the case of RuAl<sub>2</sub>, we obtained nine Wannier functions per ruthenium atom centered on each ruthenium site for the valence and a part of the conduction bands. Nine Wannier functions centered on each site can be considered as one *s*-, three *p*-, and five *d*-orbitals, which cannot straightforwardly be interpreted as atomic orbitals of the ruthenium atom but rather as those hybridized with *sp*-orbitals of neighboring aluminum atoms. Five out of seven valence bands can be associated with the five *d*-orbitals. The other two bands can be associated with bonding orbitals between *sp*<sup>3</sup>-hybrid orbitals of neighboring ruthenium atoms. It should be noted that to associate all the valence electrons with ruthenium atom indicates that formal charge of ruthenium is -6, being supported by the fact that the Born effective charge of ruthenium in RuAl<sub>2</sub> is about -6 [4].

We have confirmed that the number of the valence bands in AlIr, RuGa<sub>3</sub>, Al–Cu–Ir approximant [2], and also Al–Ir approximant known as Al<sub>11</sub>Ir<sub>4</sub> [5] can be explained as in the RuAl<sub>2</sub>. If we consider clusters centered on the sites where Wannier functions centered on, formation of the bonding orbitals can be interpreted as covalent bonds between the clusters. These covalent bonds are formed if two clusters locate at a small distance about 0.3 nm [2].

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20<sup>th</sup> September, Tuesday

## **Valence fluctuations in heavy fermion system on the Penrose lattice: real-space dynamical mean-field approach**

Ryu Shinzaki, Joji Nasu, and Akihisa Koga

*Department of Physics, Tokyo Institute of Technology 152-8551 Japan*

Heavy fermion systems with rare-earth or actinide elements have attracted considerable attention. Among them, valence fluctuations and valence transitions are some of interesting phenomena in the compounds, where the valence in rare-earth ions abruptly changes due to applied field and/or pressure. Recently, it is suggested that quantum critical behavior in the quasicrystal  $\text{Au}_{51}\text{Al}_{35}\text{Yb}_{14}$  [1] are related to valence fluctuations, which stimulates further theoretical and experimental investigations on strong correlations in the quasiperiodic systems [2-5].

Valence fluctuations and valence transitions in the conventional periodic system have been studied theoretically in terms of the extended periodic Anderson model [6]. The possibility of the valence transition in this model has been discussed by means of various theoretical approaches. However, it is still unclear whether or not the valence transition occurs even in the quasiperiodic lattice. In particular, each lattice site in the quasiperiodic system is not equivalent, which is in contrast to the conventional periodic system. Therefore, it is highly desired to clarify how the local geometry affects valence fluctuations, by taking the quasiperiodic structure into account correctly.

Motivated by this, we study the extended Anderson lattice model on the Penrose lattice to discuss valence fluctuations at low temperatures. Combining the real-space dynamical mean-field theory with the continuous-time quantum Monte Carlo method, we calculate the f-electron number, spin correlations, and local magnetic susceptibility to discuss low temperature properties characteristic of the strongly correlated electron systems on the quasiperiodic lattice.

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20<sup>th</sup> September, Tuesday

## Search for semiconducting quasicrystal and high-performance thermoelectric material

K. Kimura<sup>1</sup>, J.T. Okada<sup>2</sup>, Y. Takagiwa<sup>3</sup> and K. Kitahara<sup>1</sup>

<sup>1</sup>*The University of Tokyo, Kashiwa, Chiba 277-8561, Japan*

<sup>2</sup>*Tohoku University, Sendai, Miyagi 980-8577, Japan*

<sup>3</sup>*National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan*

The question of whether insulating or semiconducting quasicrystals exist has been a basic problem for solid state physics since the award of the Nobel Prize in 2011, which confirmed quasicrystal as being a solid-state structural phase on the same level as crystalline and amorphous phases. There have been two approaches by which to realize them. One is using boron-based systems. Boron is often classified as a non-metallic element, and it has various crystalline structures constructed from icosahedral or pentagonal clusters, some of which are classified as quasicrystalline approximants. The other approach involves aluminum–transition metal (Al–TM) icosahedral quasicrystals, in which metallic–covalent bonding conversion (MCBC) has been found to occur depending on whether a central atom inside the icosahedral clusters exists or not [1].

The icosahedral Al–Pd–TM (TM: Re, Mn) quasicrystals are considered to be an intermediate state among the three typical solids: metals, covalently bonded networks (semiconductor), and molecular solids. Using this picture, we propose a guiding principle of weakly bonded rigid heavy clusters to increase the thermoelectric figure of merit (ZT) by optimizing the bond strengths of intra- and inter-icosahedral clusters. Through element substitutions that mainly weaken the inter-cluster bonds, a dramatic increase of ZT from less than 0.01 to 0.26 was achieved. To further increase ZT, materials should form a real gap, i.e. semiconducting quasicrystal, to obtain a higher Seebeck coefficient [1].

Our recent calculation showed that the Al–Cu–Ir 1/0-cubic approximant had a semimetallic band structure, which should be qualitatively equivalent to a semiconducting one. We discuss the mechanism underlying the formation of valence bands in terms of molecular-like orbitals of clusters, and reveal what orbitals compose such valence bands. To extract such orbitals, we used the method of maximally localized Wannier functions, which is a robust way of extracting representative orbitals corresponding to a specified energy range [2].

Viscosity of liquid boron was measured over the temperature range from 2325 to 2556 K using an electrostatic levitation method combined with an oscillation drop technique. The results obtained revealed that the viscosity increases slowly with decreasing temperature above the melting temperature ( $T_m=2360$  K), and substantially increases with further decrease in temperature below  $T_m$ . The increase in the viscosity suggests that clusters with extension may appear in supercooled liquid of boron. Using rapid quenching from the supercooled state, we are searching semiconducting quasicrystal boron.

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20<sup>th</sup> September, Tuesday

## Schottky Effect in Rare-Earth-Containing Quasicrystals

Janez Dolinšek

*Jožef Stefan Institute and University of Ljubljana, Faculty of Mathematics and Physics,  
Jamova 39, SI-1000 Ljubljana, Slovenia, e-mail: jani.dolinsek@ijs.si*

The analysis of low-temperature specific heat of rare-earth (RE)-containing quasicrystals and periodic approximants and consequent interpretation of their electronic properties in the  $T \rightarrow 0$  limit is frequently hampered by the Schottky effect, where crystalline electric fields lift the degeneracy of the RE-ion Hund's rule ground state and introduce additional contribution to the specific heat. We have studied the low-temperature specific heat of thulium-containing  $i$ -Zn-Ag-Sc-Tm icosahedral quasicrystal and its 1/1 Zn-Sc-Tm approximant, both being classified as "Schottky" systems [1]. We have derived the crystal-field Hamiltonian for pentagonal symmetry of the crystalline electric field, pertinent to the class of Tsai-type icosahedral quasicrystals and their approximants, where the RE ions are located on fivefold axes of the icosahedral atomic cluster. Using the leading term of this Hamiltonian, we have calculated analytically the Schottky specific heat in the presence of an external magnetic field and made comparison to the experimental specific heat of the investigated quasicrystal and approximant. When the low-temperature specific heat  $C$  is analyzed in a  $C/T$  versus  $T^2$  scale (as it is customary done for metallic specimens), the Schottky specific heat yields an upturn in the  $T \rightarrow 0$  limit that cannot be easily distinguished from a similar upturn produced by the electron-electron interactions in exchange-enhanced systems and strongly correlated systems. Our results show that extraction of the electronic properties of RE-containing quasicrystals from their low-temperature specific heat may be uncertain in the presence of the Schottky effect.

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## Anomalous quantum diffusion in quasicrystals and approximants

G. Trambly de Laissardière<sup>1</sup>, A. Szallas<sup>2</sup>, C. Oguey<sup>1</sup> and D. Mayou<sup>3</sup>

<sup>1</sup>*Lab. Physique Théorique et Modélisation, CNRS / Univ. de Cergy-Pontoise, F-95302 Cergy-Pontoise, France*

<sup>2</sup>*Wigner Research Centre for Physics, P.O. Box 49, H-1525 Budapest, Hungary*

<sup>3</sup>*Institut Néel, CNRS / Univ. Grenoble Alpes, F-38042 Grenoble, France*

Since the discovery of quasicrystals by Shechtman et al. numerous experimental studies indicated that the conduction properties of several stable quasicrystals (AlCuFe, AlPdMn, AlPdRe...) are quite opposite to those of good metals (see for instance ref. [1]). It appears also that the medium range order, over one or a few nanometers, is a relevant length scale that determines conductivity. In particular, the role of transition elements enhancing localization has been often studied (Ref. [2] and Refs. therein). There is also strong evidence that these nonstandard properties result from a new type of breakdown of the semiclassical Bloch-Boltzmann theory of conduction [2,3]. On the other hand, the specific role of long range quasiperiodic order on transport properties is still an open question in spite of a large number of studies (Ref. [4,5] and Refs. therein).

Here, we present numerical calculations of the electronic quantum diffusion to study “how electrons propagate” in approximants of quasicrystals (AlMn, AlCuFe), and in 2-dimension quasiperiodic tilings (Penrose tiling and octagonal tiling). Our results show that both medium range and long range quasiperiodic orders induce sub-diffusive states at some energies, whereas diffusive or super-diffusive states are found at other energies. Therefore a small shift of the Fermi energy can cause a system without defects to undergo a metal-insulator transition. We present also the effect of static disorder on diffusive properties.

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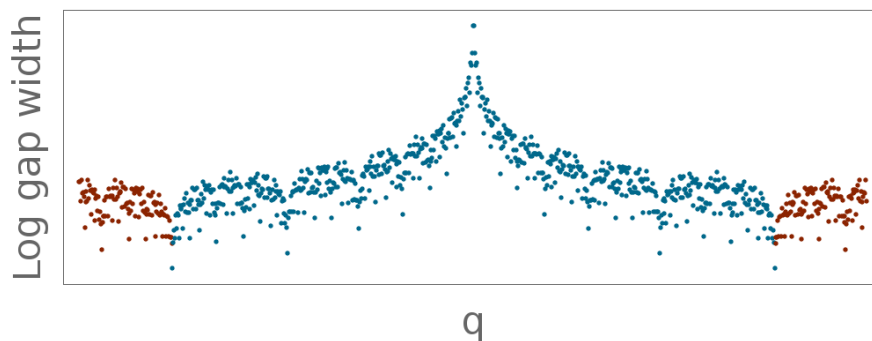
## Gap structure and topological indices on the Fibonacci quasicrystal

Nicolas Macé, Frédéric Piéchon and Anuradha Jagannathan

*Laboratoire de Physique des Solides, Université Paris-Saclay, 91400 Orsay, France.*

The unique structural properties of quasicrystals result in unusual electronic properties. The main known result in this context is the *gap labeling theorem*. It relates the integrated density of states (idos) in the gaps of the energy spectrum to the geometry of the quasicrystal. For the quasiperiodic *Fibonacci chain* for example, it states that the idos in the gaps is  $\tau q \bmod 1$  where  $q$  is an integer and  $\tau$  the golden ratio. Interestingly, the labeling does not depend on the details of the Hamiltonian we endow the quasicrystal with. In that sense,  $q$  is *topological* [1].

The gap labeling only applies to idealized, infinite quasicrystals. Based on a real-space renormalization group approach [2,3], we study how it is modified when one turns to more realistic *finite size approximants*. We show, on the example of the Fibonacci chain, that it naturally extends to these systems. Two kind of gaps come into play: the *transient gaps*, that close in the large approximant size limit, and *permanent gaps* that do not [4]. We show that the nature of a gap is intrinsically linked to the geometry of the quasiperiodic chain. Plotting gap width as a function of the gap label  $q$  reveals an interesting structure [fig. 1], hinting that  $q$  has a relevant physical meaning.



*Figure 1: Gap width as a function of the gap index  $q$ , for a pure-hopping Hamiltonian, for the approximant  $n=16$ . Permanent gaps are shown in blue, and transient gaps in red.*

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20<sup>th</sup> September, Tuesday

## Magnetism and superconductivity in icosahedral quasicrystals and approximants with Tsai-type clusters

Kazuhiko Deguchi<sup>1</sup>, Syuya Matsukawa<sup>1</sup>, Keiichiro Imura<sup>1</sup>, Noriaki K. Sato<sup>1</sup>  
and Tsutomu Ishimasa<sup>2</sup>

<sup>1</sup>*Department of Physics, Graduate School of Science, Nagoya University, Nagoya, Aichi 464-8601, Japan*

<sup>2</sup>*Division of Applied Physics, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan*

Quasicrystals possess long-range, quasi-periodic structures with diffraction symmetries forbidden to crystals. Recently, a new type of icosahedral Yb quasicrystal and approximant was discovered [1]. The Au-Al-Yb quasicrystal exhibits novel quantum critical behavior ( the divergence of the magnetic susceptibility as  $T \rightarrow 0$  ) as observed in Yb-based heavy fermion materials with intermediate Yb valence, while the Au-Al-Yb approximant shows heavy Fermi liquid behavior [2]. Furthermore, quantum critical phenomenon of the Au-Al-Yb quasicrystal is remarkably robust against hydrostatic pressure. By contrast, the Au-Al-Yb approximant shows heavy fermion behavior, very sensitive to hydrostatic pressure and quantum criticality of the approximant is induced by pressure. Therefore, the quantum critical state of the Au-Al-Yb quasicrystal might correspond to an electronic state unique to the quasicrystals. For superconductivity, there are a few reports of superconductivity in the quasicrystals to the best of our knowledge. We have found superconductivity of icosahedral Yb approximants by the substitution of Al atoms to Ge atoms in Au-Al-Yb alloys [3,4]. Until very recently, quantum criticality and superconductivity has been intensively studied in only crystalline materials: for example, heavy fermion compounds. Interestingly, quantum criticality of the Au-Al-Yb quasicrystal seems to be closely related to heavy fermion crystalline compound  $\beta$ -YbAlB<sub>4</sub> with intermediate Yb valence [5,6]. Magnetism and superconductivity in icosahedral Yb quasicrystals and approximants will be presented and discussed.

[1] T. Ishimasa, Y. Tanaka, and S. Kashimoto, *Phil. Mag.* **91**, 4218 (2011).

[2] K. Deguchi *et al.*, *Nature Materials* **11**, 1013 (2012).

[3] K. Deguchi *et al.*, *J. Phys. Soc. Jpn.* **84**, 023705 (2015).

[4] K. Deguchi *et al.*, *J. Phys. Soc. Jpn.* **84**, 015002 (2015).

[5] S. Nakatsuji *et al.*, *Nature Physics* **4**, 603 (2008).

[6] Y. Matsumoto *et al.*, *Science* **331**, 316 (2011).

20<sup>th</sup> September, Tuesday

## **Magnetic charges in quasiperiodic vertex models**

Elena Y. Vedmedenko

*Department of Physics, University of Hamburg, Hamburg, 20355 Germany*

Last years have been marked by the huge progress in experimental fabrication of two-dimensional artificial quasicrystals by means of structuring of thin ferromagnetic films [1]. The strong shape anisotropy of elements of artificial magnetic quasicrystals requires them to behave as macroscopic Ising spins. This property permits to regard these systems as quasicrystalline vertex models similar to two-dimensional artificial spin-ices.

First investigations of such artificial quasicrystalline tilings report a novel type of ordered magnetic ground state composed of four magnetic sublattices [1] similar to that found for free magnetic rotators on quasicrystalline tilings earlier [2]. Vertices of those artificial quasiperiodic tilings naturally acquire uncompensated magnetic charges [1]. The mechanism of interaction between those magnetic charges, however, is still unclear.

Here, numerical and analytical analyses of magnetic dipolar spin ice on octagonal and Penrose tiling is presented. Particular attention is paid to the evolution and the distribution of uncompensated magnetic charges as a function of external magnetic field. The results are compared with experimental data [1]. It is demonstrated that depending on the micromagnetic reversal mechanism in individual particles charge ordered states or accumulation of magnetic charges can be observed.

[1] B. Farmer, V. S. Bhat, A. Balk, E. Teipel, N. Smith, J. Unguris, D. J. Keavney, J. T. Hasting and L. E. De Long, arXiv:1501.02760, accepted to Phys. Rev. B

[2] E. Y. Vedmedenko, U. Grimm, and R. Wiesendanger, Phys. Rev. Lett. **93**, 076407 (2004).

## Local and short-range electron correlation effects on the Penrose lattice

Nayuta Takemori<sup>1</sup>, Akihisa Koga<sup>2</sup> and Hartmut Hafermann<sup>3</sup>

<sup>1</sup>*Center for Emergent Matter Science, RIKEN, Wako, 351-0198, Japan*

<sup>2</sup>*Department of Physics, Tokyo Institute of Technology, Meguro-ku, Tokyo, 152-8551, Japan*

<sup>3</sup>*Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co. Ltd., Boulogne-Billancourt, 92100, France*

Strong electron correlations in quasiperiodic systems have attracted much interest since the recent observation of quantum critical behaviour in the Tsai-type quasicrystal compounds  $\text{Au}_{51}\text{Al}_{34}\text{Yb}_{15}$  [1]. To clarify how electron correlations affect low temperature properties in quasiperiodic systems, we study the repulsive Hubbard model on the Penrose lattice. Using the real-space dynamical mean-field theory (RDMFT) [2] to investigate local electron correlations, we clarify that the quasiparticle weight strongly depends on the lattice site and its geometry when the system is close to the Mott transition point. Moreover, we find a temperature dependent distribution of local quantities characteristic of the Penrose lattice [3]. This behaviour originates from the local isomorphism which holds high geometrical regularity even if there are no translational symmetry. Moreover, we extend the dual fermion approach [4] to real-space description [5] for investigating intersite electron correlations in inhomogeneous lattices and clarify that the Mott transition point appears at relatively high temperatures compared to the crossover point obtained by the RDMFT method since short-range antiferromagnetic fluctuations lower the density of states at Fermi level sufficiently to form the Mott insulator. This fact is consistent with results obtained by the real-space dual fermion approach in homogeneous lattices. We also clarify that the site-dependence of local quantities is enhanced by taking local and short-range correlations into account. This indicates that the site-dependent renormalization is much enhanced by inducing longer-range correlation effects in the Penrose lattice. Our study clarifies how local and nonlocal electron correlations affect the local quantities in the quasiperiodic system and offers new powerful method for investigating low temperature properties of strongly correlated electron systems on inhomogeneous lattices.

[1] K. Deguchi., et al., *Nat. Mater.* **11**, 1013-1016 (2012)

[2] A. Georges et al., *Rev. Mod. Phys.* **68**, 13 (1996).

[3] N. Takemori, and A. Koga., *J. Phys. Soc. Jpn.* **84**, 023701 1-5 (2015); N. Takemori, and A. Koga., *J. Phys.: Conf. Ser.* **592** 012038 (2015)

[4] A. N. Rubtsov et al., *Phys. Rev. B* **77**, 033101 (2008).

[5] N. Takemori, A. Koga and H. Hafermann, *J. Phys.: Conf. Ser.* **683** 012040 (2016).

20<sup>th</sup> September, Tuesday

## Phenomenological magnetic model in Tsai-type approximants

Takanori Sugimoto<sup>1</sup>, Takami Tohyama<sup>1</sup>, Takanobu Hiroto<sup>2</sup>, and Ryuji Tamura<sup>3</sup>

<sup>1</sup>*Department of Applied Physics, Tokyo University of Science, Tokyo 125-8585, Japan*

<sup>2</sup>*Department of Advanced Material Science, University of Tokyo, Chiba 277-8561, Japan*

<sup>3</sup>*Department of Material Science and Technology, Tokyo University of Science, Tokyo 125-8585, Japan*

Recent neutron diffraction study has reported a curious ferromagnetism in Tsai-type approximants Au-Si-RE (RE = Gd, Tb, Dy, and Ho) [1] and Au-Al-RE [2], which have the same local structure as quasi-crystals with a translational symmetry simultaneously. In these materials, magnetic moments of rare-earth atoms have a single-ion anisotropy determined locally via spin-orbit coupling around crystal fields satisfying a distorted icosahedral crystal structure. We phenomenologically propose a possible magnetic model reproducing the magnetic structure and the thermodynamical quantities. The corresponding energies of the single-ion anisotropy and RKKY exchange couplings are also estimated by comparing magnetization curves and susceptibility of our model and experiments. Moreover, simulated annealing calculations with the energies in our model coincide with the strange ferromagnetism. In conclusion, a local symmetry of icosahedral cluster in body-centered cubic structure plays a key role to exhibit the peculiar magnetic structure [3]. Our magnetic model does not only explain magnetic behaviors in quasi-crystal approximants, but also can approach to a coexistence of a long-ranged order and a quasi-periodicity.

[1] T. Hiroto, T. J. Sato, H. Cao, and R. Tamura, to be published; T. Hiroto, PhD thesis, Tokyo Univ. Sci. (2015).

[2] A. Ishikawa, T. Hiroto, K. Tokiwa, T. Fujii, and R. Tamura, Phys. Rev. B **93**, 024416 (2016).

[3] T. Sugimoto, T. Tohyama, T. Hiroto, and R. Tamura, J. Phys. Soc. Jpn. **85** 053701 (2016).



20<sup>th</sup> September, Tuesday

## Magnetic order in $RCd_6$ single crystals – the approximants to the spin-glass $i$ - $R$ -Cd quasicrystals

Andreas Kreyssig<sup>1</sup>, Benjamin G. Ueland<sup>1</sup>, Jens-Uwe Hoffmann<sup>2</sup>,  
Guillaume Beutier<sup>3</sup>, Marc de Boissieu<sup>3</sup>, and Alan I. Goldman<sup>1</sup>

<sup>1</sup>*Ames Laboratory and Dept. of Physics and Astronomy, Iowa State University, Ames, USA*

<sup>2</sup>*Helmholtz-Zentrum Berlin, Germany*

<sup>3</sup>*Univ. Grenoble Alpes & CNRS, SIMAP, Grenoble, France*

Since the discovery of quasicrystals, there has been an intense search for magnetic ordering in aperiodic structures. The recently discovered  $i$ - $R$ -Cd quasicrystals and  $RCd_6$  approximants offer a set of model systems for attaining a deeper understanding of how the magnetism evolves from a conventional lattice in the approximant phase to an aperiodic quasicrystal given the chemical simplicity associated with binary compounds. X-ray resonant magnetic scattering studies demonstrated that the  $RCd_6$  approximants show long-range magnetic order with the rare-earth ( $R$ ) magnetic moments antiferromagnetically correlated between the two quasi-icosahedral clusters related through the body-center symmetry of the cubic unit cell [1, 2]. In contrast, magnetization measurements show in  $i$ - $R$ -Cd quasicrystals that the  $R$  magnetic moments freeze spin-glass like at low temperatures [3].

Here we present neutron diffraction studies of the magnetic order in the  $TbCd_6$  approximant possible by the usage of  $^{112}Cd$  isotope avoiding the strong neutron absorption by natural Cd and revealing a more complex magnetic ordering. Magnetic resolution-limited Bragg peaks have been not only observed at positions related to the propagation vector (0 0 1) in notation of the body-centered cubic unit cell as previously reported, but also at positions that can be indexed by a propagation vector of  $(\frac{1}{2} \frac{1}{2} 0)$  corresponding to the "superstructure-component" of the cubic-to-monoclinic transition developing at higher temperature caused by the orientational ordering of the inner Cd tetrahedral in the center of each quasi-icosahedral cluster. Surprisingly, single crystals without post-annealing and studied only few days after growing them showed a more complex magnetic order with dominating magnetic Bragg peaks at incommensurate positions besides the previously observed magnetic Bragg peaks in single crystals and powders undergoing post-annealing. This highlights the sensitivity of the magnetic ordering to small energy-scale effects like possible disorder and points to weak or frustrated magnetic interactions in these compounds.

[1] M. G. Kim *et al.*, Phys. Rev. B **85**, 134442 (2012). [2] A. Kreyssig *et al.*, Phil. Mag. Lett. **93**, 512 (2013). [3] A. I. Goldman *et al.*, Nature Mat. **12**, 717 (2013).

20<sup>th</sup> September, Tuesday

## Neutron-scattering study on the quasicrystal approximants Au-Si-R (R = rare-earths)

Takanobu Hiroto<sup>1</sup>, Taku J. Sato<sup>2</sup>, Huibo Cao<sup>3</sup>, Kaoru Kimura<sup>1</sup> and Ryuji Tamura<sup>4</sup>

<sup>1</sup> Graduate School of Frontier Sciences, the University of Tokyo, 277-8561, Japan

<sup>2</sup> Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 980-8577, Japan

<sup>3</sup> Quantum Condensed Matter Division, Oak Ridge National Laboratory, 37831, USA

<sup>4</sup> Department of Materials Science and Technology, Tokyo University of Science, 125-8585 Japan  
hiroto@phys.mm.t.u-tokyo.ac.jp

After the discovery of icosahedral quasicrystal (*i*-QC), the existence of long-range magnetic ordering of *i*-QCs is hidden in a veil of mystery to be elucidated in materials science and physics. By contrast, various magnetic orders discovered in Tsai-type approximants [1-4] can become a good experimental starting point for a realization of *quasiperiodic magnetic order*.

In this presentation, we report the magnetic structure of Au-Si-Tb approximant based on the single crystal neutron magnetic scattering experiment. The overall magnetic structure is described as follows: four Tb<sup>3+</sup> magnetic moments on a same {1 0 0} plane are aligned along the <0 1 0> direction and exhibit a net magnetic moment toward the <1 1 1> direction. This *unique* magnetic structure is possible when the relatively strong uniaxial anisotropy, originate from the crystal fields around R<sup>3+</sup> ions (site symmetry; *m*) rather than RKKY interaction.

We will also present the effect of crystal field effect for the magnetic structure of the Au-Si-R approximants.

[1] R. Tamura *et al.*, *Phys. Rev. B* **82** (2010) 220201(R).

[2] T. Hiroto *et al.*, *J. Phys.: Condens. Matter* **25** (2013) 426004.

[3] T. Hiroto *et al.*, *J. Phys.: Condens. Matter* **26** (2014) 216004.

[4] A. Ishikawa *et al.*, *Phys. Rev. B* **93** (2016) 023316.

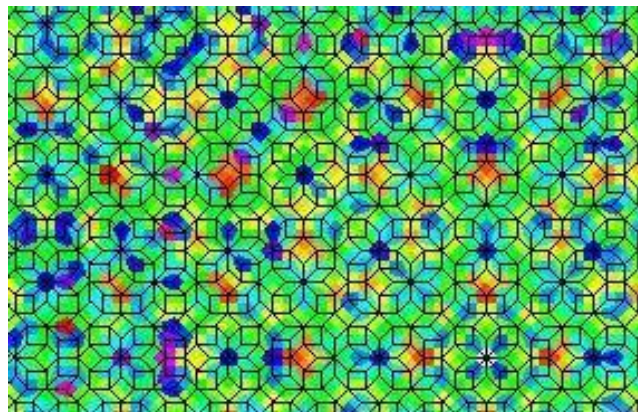
## Screening of magnetic impurities in quasicrystals

Anuradha Jagannathan

*Laboratoire de Physique des Solides, Université Paris-Sud,*

*91405 Orsay, France*

I will present some results of numerical studies on the screening of magnetic impurities in metallic quasicrystals. The studies were motivated by experimental observations of non Fermi liquid behavior in a heavy fermion quasicrystal [1], which raised the question of the possible role played by critical states, if they exist, in quasicrystals. In our recent investigations [2], we considered conduction electrons on approximants of a quasiperiodic tiling interacting with a single local moment which is described in terms of the  $U \rightarrow \infty$  Anderson impurity model. Introducing two variational parameters the resulting saddlepoint equations for the free energy are solved numerically. The distributions of Kondo temperatures  $P(T_K; \mu, J)$  was obtained by varying the position of the impurity at fixed chemical potential  $\mu$  for different values of the Kondo coupling parameter  $J$ . The distributions were found to be divergent as  $T_K$  goes to zero, indicating that, in the dilute alloy system, a considerable fraction of moments should remain unquenched down to very low temperatures. This should lead to non Fermi liquid behavior and divergence of the magnetic susceptibility of the system. We checked that these predictions extend to the case of three dimensional icosahedral tiling. Our theoretical understanding for the nature of electronic states and the origin of this type of singular behavior will be discussed.



*Figure: wavefunction amplitudes close to the main pseudogap for the octagonal tiling (detail)*

[1] K. Deguchi et al, Nat.Mater. 11, 1013(2012) ; T. Watanuki et al, Phys.Rev.B 86, 094201 (2012).

[2] E. C. Andrade, A. Jagannathan, E.Miranda, M. Vojta, V. Dobrosavljevic, Phys.Rev.Lett. 115, 036403 (2015).

20<sup>th</sup> September, Tuesday

## Magnetic properties of Au-based Tsai-type approximants

R. Tamura<sup>1</sup>, A. Ishikawa<sup>1</sup>, T. Seki<sup>2</sup>, N. Shibata<sup>2</sup>

<sup>1</sup>*Department of Mater. Sci. & Tech., Tokyo University of Science, Niijuku, Katsusika-ku, Tokyo 125-8585, Japan*

<sup>2</sup>*Institute of Engineering Innovation, The University of Tokyo, Yayoi, Bunkyo-ku, Tokyo 133-8656, Japan*

In 2010, a long-range antiferromagnetic (AFM) order was found in the Cd<sub>6</sub>Tb approximant [1] and since then both AFM and ferromagnetic (FM) orders have been observed in various Tsai-type approximants, in addition to conventional spin-glass-like behaviors. The origin of such different behaviours has now become an interesting issue. In this work, we have replaced Cd by Au and Al in Cd<sub>6</sub>Gd and found that Au and Al are mutually replaced more than 23 at %. Thus, the Au-Al-Gd system has become an ideal system for investigating the role of another freedom, i.e., the valence electron freedom, in the magnetic behaviour of Tsai-type approximants. The change in the Au/Al ratio in Au-Al-Gd leads to an oscillation of the Weiss temperature, which is accounted for by a continuous change of the Fermi wave vector  $k_F$  [2]. When the Weiss temperature is large positive, i.e., FM contributions are dominant, a FM order appears at the lowest temperature. On the other hand, reducing the Weiss temperature likely leads to a spin-glass-like behaviour, which is understood as a consequence of the interplay between AFM contributions and randomness. Detail of the magnetic behaviours in the Au-Al-Gd approximant will be discussed also with the results of STEM observations.

[1] R. Tamura *et al.*, *Phys. Rev. B.* 82, 220201(R) (2010).

[2] A. Ishikawa *et al.*, *Phys. Rev. B* 93, 024416 (2016).

## Equivalence classes of Fibonacci lattices and their similarity properties

Nicolino Lo Gullo<sup>1,3</sup>, Laura Vittadello<sup>2</sup>, Luca Dell'Anna<sup>2,3</sup>, and Marco Bazzan<sup>2,3</sup>

<sup>1</sup>*Department of Physics, Università degli Studi di Milano, Milano, Italy*

<sup>2</sup>*Department of Physics, Università degli Studi di Padova, Padova, Italy*

<sup>3</sup>*CNISM, Padova Unit, Padova, Italy*

Fibonacci lattices are the paradigm of one-dimensional quasiperiodic crystals and are perhaps the most studied instance of quasiperiodic order. These lattices are such that the relative distance between adjacent points can take on only two values, namely L (long) and S (short), and their occurrence along the lattice is in accordance with the Fibonacci strings. An usual assumption is that the ratio  $L/S = (\sqrt{5} + 1)/2$ , namely the golden ratio. This implies that the lattice is self-similar under proper scaling [1].

In our work we study the scaling properties of Fibonacci lattices allowing for ratio  $L/S$  to be any real number and show that through the concept of composition on Fibonacci strings it is possible to define classes of equivalence for these generalized Fibonacci lattices. After defining the classes of equivalence we show that they are meaningful from both the static and dynamical point of view. By means of the Kullback-Leibler divergence we show that the diffraction patterns of two Fibonacci lattices are similar only if they belong to the same class of equivalence.

We also compare the theoretical diffraction spectra with the spectra obtained from the diffraction of light on gratings of optical waveguides in lithium-niobate finding again that two Fibonacci lattices are similar only if they belong to the same equivalence class (Figure 1). In this case diffraction spectra encompass a structure factor due to the shape of the single waveguides and it is by no means trivial that the scaling properties of the diffraction spectra are still maintained.

We then move to consider the energy spectrum of a particle moving in a one-dimensional potential with minima of same depth but whose positions on the line are distributed according to the Fibonacci lattices. We show that the opening of energy gaps (with respect to the free case) occurs at the same momenta for Fibonacci lattices belonging to the same equivalence class. This result is useful in the spirit of the gap labeling theorems and in particular to the labeling of gaps by selecting the brightest peaks in the diffraction patterns of quasicrystals [2].

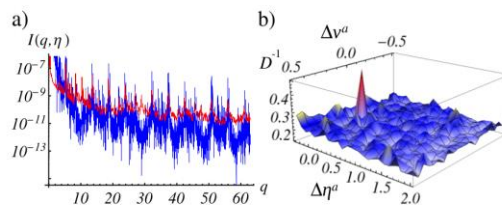


Figure 1: a) Experimental diffraction pattern (solid red curve) for a Fibonacci grating with  $N = 300$  lines and  $L = 23 \mu\text{m}$  and  $S = 17 \mu\text{m}$ , compared with the theoretical diffraction pattern with the inclusion of the structure factor (solid blue curve). b) The inverse of KL divergence between the experimental data and the theoretical diffraction spectra of different FLs. The maxima (minima of  $D$ ) occurs when the two FLs belong to the same equivalence class.

[1] M. Senechal, Quasicrystals and geometry, Cambridge University Press (1995).

[2] J.-M. Gambaudo, and P. Vignolo, New J. Phys. 16, 043013 (2014).

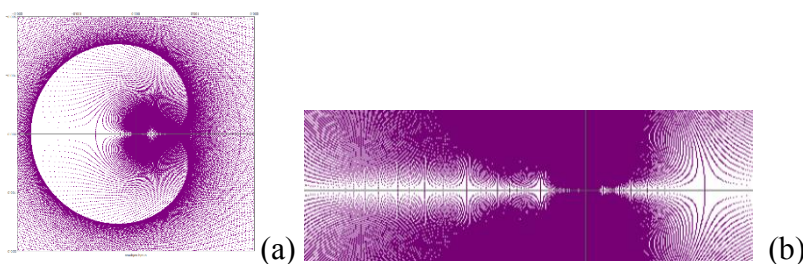
## Fractality in quasicrystals and prime number distribution

Fang Fang and Klee Irwin

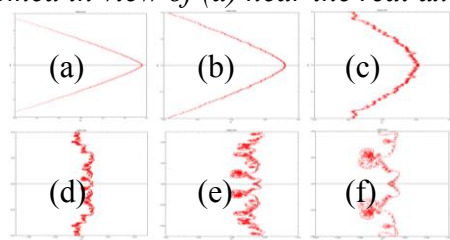
*Quantum Gravity Research, Los Angeles, CA, USA*

The scale-invariant self-similarity of quasicrystals gives them fractal properties [1] and makes them fractal in nature [2]. In exploring the Fibonacci chain, we discovered a new fractal pattern in the complex space of its Fourier transform (Fig. 1). Using the box-counting method, its fractal dimension is calculated to be about  $2/3$ .

Using the same method, we generated a fractal-like pattern in the complex space of the Fourier transform of the logarithm of the prime numbers. (Fig. 2). Its fractal dimension, using the box-counting method, is about 0.56. This result supports Freeman Dyson's conjecture that prime numbers and the associated non-trivial zeros of the Zeta function in the Riemann Hypothesis are ordered as a 1D quasicrystal [3]. It is also in line with the work of Andrew Odlyzko, who published the Fourier transform of the Zeta-function zeros, showing sharp discontinuity at every logarithm of a prime or prime-power number and nowhere else – a hallmark of the inherent order of crystals and quasicrystals [4].



*Figure 1: Fractal pattern in the complex space of the Fourier transform of the Fibonacci chain with 25 iterations. (b) is a zoomed in view of (a) near the real axis.*



*Figure 2: Fractal-like pattern in the complex space of the Fourier transform of the logarithm of the prime numbers - zooming in from (a) to (f).*

- [1] E.L. Albuquerque, and M.G. Cottam, Theory of elementary excitations in quasiperiodic structures, *Physics Reports* **376**, 225-337 (2003).
- [2] P. Ramachandrarao, A. Sinha, and D. Sanyal, *Current Science* **79**, 364-366 (2000).
- [3] F. Dyson, *Birds and Frogs*, *Notices of the AMS* **56**, 212-223 (2009).
- [4] A.M. Odlyzko, *Primes, quantum chaos and computers*, in *Number Theory*, Proceedings of a Symposium, National Research Council, Washington DC, 35–46 (1990).

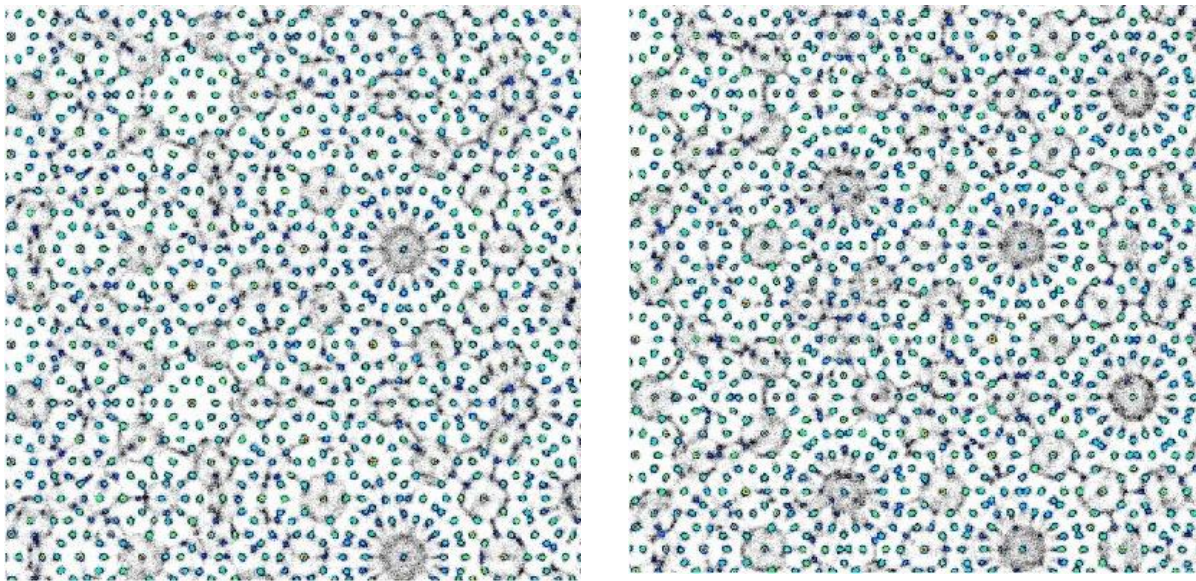
## Finite temperature structure and stability of i-AlCuFe and i-AlMnPd from realistic simulations

Marek Mihalkovič<sup>1</sup> and Michael Widom<sup>2</sup>

<sup>1</sup>*Institute of Physics, Slovak Academy of Sciences, Dubravská cesta 9, 84511 Bratislava, Slovakia*

<sup>2</sup>*Department of Physics, Carnegie Mellon University, 5000 Forbes Ave., Pittsburgh, PA 15213, USA*

Empirical oscillating pair potentials [1] fitted to ab-initio data provide for a unique setup making possible studies of formation and stability of the fundamental icosahedral phases, i-AlMnPd and i-AlCuFe. Firstly, we obtain unbiased structural insights by crystallizing ternary melts in unit cells with magic "2/1" and "3/2-2/1-2/1" sizes (12.2Å and 19.6x12.2x12.2Å respectively). Annealing preliminary starting structures (Katz-Gratias model or decoration of canonical cell tiling) at high temperatures above 1000K we obtain equilibrated samples of large approximants (see Fig.1) up to "8/5" (~51 or ~54Å side cubic box with 9700 atoms for i-AlCuFe and i-AlMnPd respectively). Equilibration is achieved by reshuffling networks of (defective) fundamental clusters. Slow cooling simulations then lead to low-temperature structures that were competitive with known ordinary crystalline ordinary crystalline phases, as verified by ab-initio total energy calculations for sample sizes up to ~3000 atoms (5/3 approximant). Finally we evaluate free energies of the approximants and competing crystals at finite temperatures and compute corresponding phase diagrams.



*Figure 1: Atomic occupancy integrated over two subsequent 1ns time frames in 5/3 i-AlCuFe approximant at 1140K. View parallel to pseudo-5-fold axis, 4Å thick slice.*

[1] M. Mihalkovic and C. L. Henley, Phys. Rev. B 85, 092102, 2012

## Canonical-cell icosahedral quasicrystals?

Nobuhisa Fujita

*Institute of Multidisciplinary Research for Advanced Materials,  
Tohoku University, Sendai 980-8577, Japan*

It remains to be controversial whether the canonical-cell geometry initiated by C. L. Henley [1] could describe the quasiperiodic arrangement of clusters in icosahedral quasicrystals. This clearly raises the question as to the possibility that the canonical cells can tile the three-dimensional space in a quasiperiodic and icosahedral manner.

Attempting to prove the existence of such a tiling, I have recently found a substitution rule for the canonical cells that can surely generate a quasiperiodic canonical-cell tiling [2]. This substitution rule uses the cube of the golden mean as the scaling ratio, while the canonical cells are supposed to be classified into sixteen distinct types according to their shapes and surrounding environments; each type of cell is substituted in a unique manner. It is shown that the quasiperiodic tiling thus obtained does not conform to the full icosahedral group  $-5-32/m$  but instead to its proper subgroup  $m-3$ . A peculiarity of the tiling is observed also in its Fourier transform, which exhibits a set of satellite peaks at midpoints of main peaks. These satellite peaks are attributed to a super-lattice ordering with index 4, and correspondingly the supporting module (i.e., the P-type icosahedral module) of the vertices is classified into four sub-modules for which the atomic surfaces are defined separately.

A search for a quasiperiodic tiling with the full icosahedral symmetry is still under way. The latest progress will be presented at the ICQ13.



*Figure: (left) The canonical cells. (right) A section of the quasiperiodic tiling.*

[1] C. L. Henley, Phys. Rev. B **43**, 993 (1991).

[2] N. Fujita, in preparation.

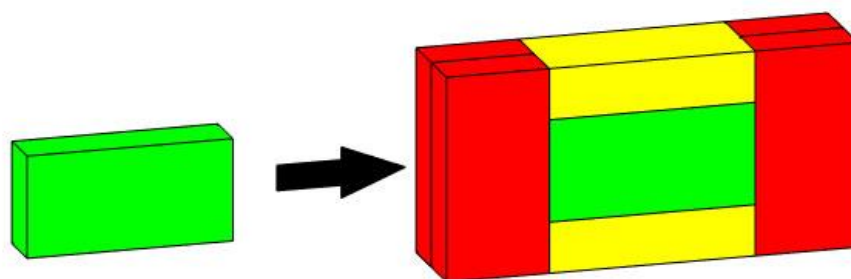


## Brick tiling

Shelomo I. Ben-Abraham and Dvir Flom

*Department of Physics, Ben-Gurion University, IL-8410501 Beer Sheba, Israel*

We present a three-dimensional analog of the two-dimensional table tiling [1] – a *brick tiling*. Its prototiles are standard bricks (henceforth "protobricks"), i.e. cuboids with edges of  $2^0 = 1$ ,  $2^1 = 2$ ,  $2^{d-1} = 2^2 = 4$  units ( $d$  for dimension). They consist of  $2^{(d-1)d/2} = 2^{2 \times 3/2} = 2^3 = 8$  basic cubes and come in  $d! = 3! = 6$  orientations. A 3D brick is a *rep-tile*, i.e. a polyhedron that can be nontrivially tiled by smaller, congruent copies of itself. Thus it induces the inflation shown in Figure 1. Moreover, we have devised a code identifying the basic cubes by  $6 \times 8 = 48$  "colors" and constructed a lattice substitution tiling that reproduces the brick tiling. We also discuss possible generalizations to arbitrary dimensions. Our companion poster [2] shows the details of the brick tiling and its "color" code tiling.



*Figure 1: Three-dimensional brick inflation.*

[1] E. A. Robinson Jr., *Indag. Mathem. N.S.* **10**, 581 (1999).

[2] D. Flom and S. I. Ben-Abraham, *"Color"code for the brick tiling*, poster at this meeting (2016).

## **Quasicrystalline phase Coxeter pairs, Ammann patterns and Penrose-like tilings**

Latham Boyle<sup>1</sup> Paul J. Steinhardt<sup>1,2,3</sup>

<sup>1</sup>*Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada*

<sup>2</sup>*Princeton Center for Theoretical Science, Princeton University, Princeton, NJ, 08544 USA*

<sup>3</sup>*Department of Physics, Princeton University, Princeton, NJ, 08544 USA*

We identify a precise geometric relationship between: (i) certain natural pairs of irreducible reflection groups ("Coxeter pairs"); (ii) self-similar quasicrystalline patterns formed by superposing sets of 1D quasi-periodically-spaced lines, planes or hyper-planes ("Ammann patterns"); and (iii) the tilings dual to these patterns ("Penrose-like tilings"). We use this relationship to obtain all irreducible Ammann grids and their dual Penrose-like tilings, along with their key properties (including their self-similarity or "inflation" rules) in a simple, systematic and unified way. In particular, we present the complete set of minimal Ammann patterns and Penrose-like tilings (six in 2D, five in 3D and one in 4D), most of which are new. We also complete the enumeration of the quasicrystallographic space groups corresponding to the irreducible non-crystallographic reflection groups, by showing that there is a unique such space group in 4D (with nothing beyond 4D).

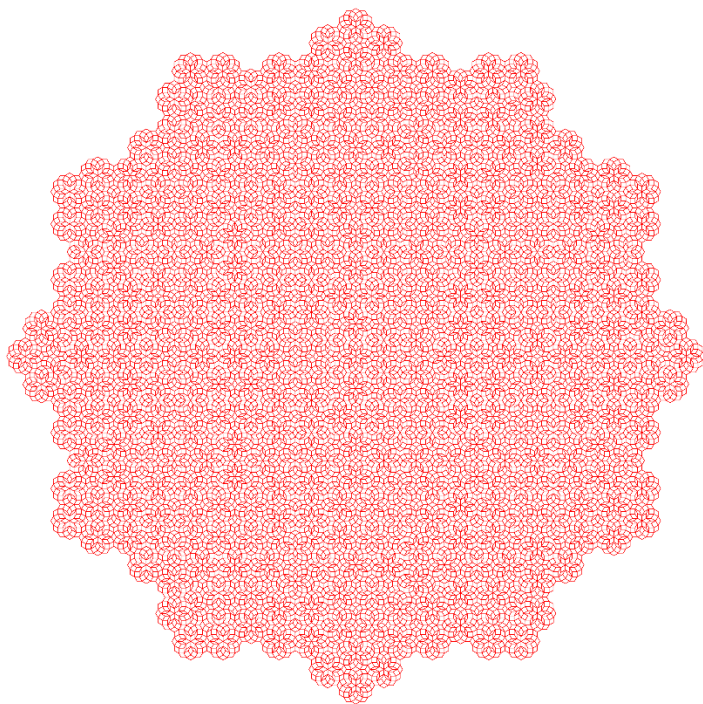
## An ancient rule for constructing dodecagonal quasi-periodic formations

Rima Ajlouni

*School of Architecture, University of Utah, Salt Lake City, UT 84112, USA*

The discovery of dodecagonal quasi-periodic patterns in historical Islamic architecture [1] is generating a renewed interest into understanding the mathematical principles of traditional Islamic geometry. Astonishingly, many centuries before its description in the modern science, ancient artists, by using the most primitive tools (a compass and a straight edge), were able to construct patterns with quasi-periodic formations [2,3,4]. Derived from these principles, a global multi-level structural model is proposed that is able to describe the global long-range order of dodecagonal quasi-periodic formations in Islamic Architecture.

This method can be used as a general guiding principle for constructing infinite patches of dodecagon-based quasi-periodic formations, without the need for local strategies (tiling, matching, grid, substitution, etc.) or complicated mathematics; providing an easy tool for scientists, mathematicians, teachers, designers and artists, to generate and study a wide range of dodecagonal quasi-periodic formations.



*Figure 1: Dodecagonal quasi-periodic pattern constructed by the author.*

[1] E. Makovicky, E. & N. Makovicky, *J. Appl. Cryst.* **44**, (2011), p. 569.

[2] R. Al Ajlouni, *Acta Crystallographica Sec. A*, **68** (2012), p. 235.

[3] R. Al Ajlouni, *Philosophical Magazine*. **91** (2011), p. 2728.

[4] R. Al Ajlouni in "Aperiodic Crystals", eds. Siegbert Schmid, Ray L. Withers, and Ron Lifshitz, Springer: Amsterdam. (2013)

## **Technological Entrepreneurship - Key to World Peace and Prosperity**

Dan Shechtman

*Technion, Haifa, Israel*

*ISU, Ames, Iowa, USA*

Over the past several decades we witness a shift toward national policies that encourage innovation and technological entrepreneurship. The call for more investment in entrepreneurship echoes around the globe as it becomes clear that except for a few countries, natural resources like oil and minerals are not enough to sustain economies, while human ingenuity is indeed the most important, sustainable natural resource.

So, is there hope for everybody on the globe to improve their lives? Can technological entrepreneurship be motivated and taught so that generations of determined entrepreneurs will build up thriving economies? The clear answer to both questions is yes and it all starts with education in general and scientific-technical education in particular. This is a long process, but there is a way to expedite it – start with the already educated engineers and scientists. These are the first candidates to open entrepreneurial endeavors. They can make the difference, but need motivation, instruction and encouraging economic environment that fosters creation of successful start-ups. These pioneering entrepreneurs can then serve as role models to others. The name of the game is motivation. If this nucleus of capable people are motivated toward entrepreneurship, a process can start that will make a huge difference in a life of a country. Living examples to countries that underwent this process are China, Israel and Singapore whose societies shifted from agrarian to industrial within several decades thanks to the spirit of entrepreneurship and the motivation to create high-tech industries led and guided by individual engineers and scientists.

In my talk I will explain the need for technological entrepreneurship and describe my involvement in turning Israel into a startup nation.

## First surface structure determination of a quasicrystalline approximant using combined surface x-ray diffraction and ab initio calculations

É. Gaudry<sup>1</sup>, C. Chatelier<sup>1</sup>, R. Felici<sup>2,3</sup>, J. Drnec<sup>2</sup>, M. de Boissieu<sup>4,5</sup>, G. Beutier<sup>4,5</sup>, L. Serkovic Loli<sup>1</sup>, G. McGuirk<sup>1</sup>, M.-C. de Weerd<sup>1</sup>, J. Ledieu<sup>1</sup>, V. Fournée<sup>1</sup>

<sup>1</sup>*Institut Jean Lamour, CNRS Université de Lorraine – UMR 7198, Nancy, France*

<sup>2</sup>*ESRF, Grenoble, France*

<sup>3</sup>*CNR-SPIN, Area della ricerca di Tor Vergata, Via del fosso del cavaliere 100, Roma, Italy*

<sup>4</sup>*Université Grenoble Alpes, Simap, Grenoble, France*

<sup>5</sup>*CNRS Simap, Grenoble, France*

Because of their large crystal cells, generally described as clusters assembly, the determination of quasicrystalline approximant surface structure is a challenging task. It results from the interplay between the selection of specific atomic planes at the surface and the preservation of atomic clusters up to the surface. Moreover, surface segregation and interatomic relaxations also play a role to decrease the surface energy.

In this work, we re-investigate the pseudo-10fold surface of the Al<sub>13</sub>Co<sub>4</sub> complex intermetallic compound (Fig. 1 left) [1,2], considered as a decagonal approximant, using both surface x-ray diffraction (SXR) and density functional theory (DFT) calculations. SXR has the advantage compared to dynamical low-energy electron diffraction (LEED-IV) that one can generally ignore multiple scattering, which makes data analysis more straight-forward. The determination of the surface structure by SXR was only possible due to the large experimental dataset which could be recorded at ESRF – the largest experimental dataset ever analyzed with this technique – a consequence of the high density of crystal truncation rods and of the relatively low symmetry of the system.

Fits of the SXR data allowed to discriminate among various surface models and pointed towards a bulk truncated surface at dense Al-rich puckered planes where protruding surface Co atoms are missing. Surface relaxations and exact atomic positions obtained by SXR and complementary DFT calculations are very similar and give confidence in the analysis. In addition, the surface energy of the corresponding surface model could be estimated from DFT calculations with a rather low value of 1.09 J/m<sup>2</sup>. This in turn allowed us to estimate interfacial energy differences, consistent with a complex interface structure. This study opens new perspectives for the determination of complex surface structures, such as quasicrystalline and related intermetallic surfaces.

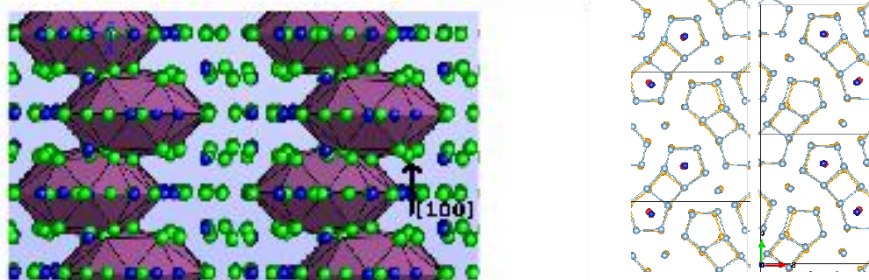


Figure 1 – Left: Crystal structure of Al<sub>13</sub>Co<sub>4</sub> highlighting Henley-type clusters. Right: Comparison of positions of surface atoms deduced from SXR (blue) and DFT (red-orange).

[1] H. Shin *et al.*, Phys. Rev. B **84**, 085411 (2011)

[2] M. Krajci and J. Hafner, J. Catal. **278**, 200 (2011)

## Structural investigation of the Al<sub>13</sub>Ru<sub>4</sub>(010) surface

Julian Ledieu<sup>1</sup>, Peter Gille<sup>2</sup>, Émilie Gaudry<sup>1</sup>, and Vincent Fournée<sup>1</sup>

<sup>1</sup> Institut Jean Lamour, UMR 7198 CNRS-Université de Lorraine, 54011 Nancy, France

<sup>2</sup> Department of Earth and Environmental Sciences, Crystallography Section, Ludwig-Maximilians-Universität München, Theresienstrasse 41, D-80333 München, Germany

Recently, quantum chemical calculations performed on several types of Al-TM (TM=Cu, Co, Fe...) complex metallic alloys have highlighted the existence of specific covalent interactions within the bulk [1,2]. In the case of the Al<sub>13</sub>TM<sub>4</sub> systems, this has led to a better understanding of their physical properties and to a description of their structure as 3-D cage compounds [2]. While well identified in the bulk materials, question arises on how these chemical bonding networks will affect the atomic structure of CMA surfaces.

To this end, the m-Al<sub>13</sub>Fe<sub>4</sub>(010) surface has been thoroughly investigated using experimental and *ab initio* methods [3]. It consists of an incomplete puckered layer where only intact clusters have been preserved, hence leading to a highly corrugated surface of low density [3]. To further understand the role of TM element among *isostructural* Al<sub>13</sub>TM<sub>4</sub> intermetallics, a m-Al<sub>13</sub>Ru<sub>4</sub> single crystal has been recently grown using Czochralski method from an Al-rich solution. Contrary to the previous system, a superstructure is observed at the Al<sub>13</sub>Ru<sub>4</sub>(010) surface using low energy electron diffraction technique. Scanning tunnelling microscopy measurements demonstrate that the superstructure consists of a network of well-separated lines running across terraces and appearing as ‘ditch’. The latter have been observed for annealing temperature ranging from 873 K to 1130 K. Within the ‘ditch’, bipentagonal motifs have been identified and resembles those observed on the Al<sub>13</sub>Fe<sub>4</sub>(010) surface, i.e. the topmost surface layer is once more related to a puckered plane present within the Al<sub>13</sub>Ru<sub>4</sub> bulk structure. Following recent reports for the Al<sub>13</sub>Fe<sub>4</sub> compound [4], we will discuss the potential catalytic properties of the Al<sub>13</sub>Ru<sub>4</sub>(010) surface based on the site-isolation concept [5].

[1] Y. Grin, et al., *J. Solid State Chem.* 179, 1707 (2006)

[2] P. Jeglič, et al., *Phys. Rev. B* 82, 104201 (2010)

[3] J. Ledieu, et al., *Phys. Rev. Lett.*, 110 (2013) 076102

[4] M. Armbrüster, et al., *Nature Materials* 11, 690 (2012)

[5] K. Kovnir, et al., *Science and Technology of Advanced Materials* 8, 420 (2007)

## Self-assembling of 5-fold symmetric molecules on quasicrystalline surfaces.

Nataliya Kalashnyk<sup>1</sup>, Émilie Gaudry<sup>1</sup>, Julian Ledieu<sup>1</sup>, C. Cui<sup>2</sup>, An-Pang Tsai<sup>3</sup>,  
Vincent Fournée<sup>1</sup>

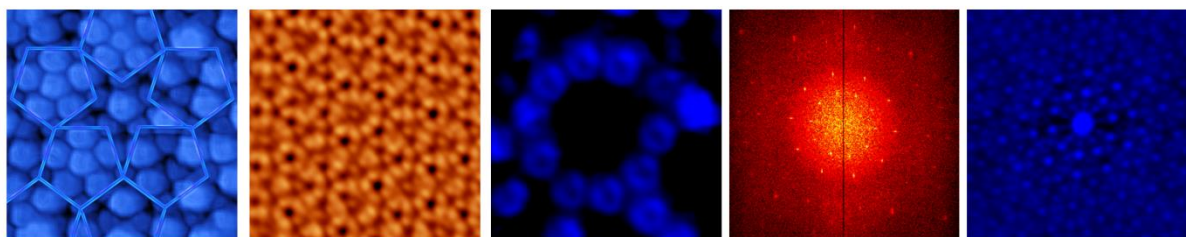
<sup>1</sup>*Institut Jean Lamour, UMR 7198 CNRS – Université de Lorraine, Nancy, FRANCE*

<sup>2</sup>*Department of Physics, Zhejiang Sci-Tech University, Hangzhou 310018, CHINA.*

<sup>3</sup>*IMRAM, Tohoku University, Sendai, JAPAN.*

The surface of quasicrystals and their approximants usually terminates at specific planes of the bulk structure. The selected terminations depend on several parameters like their chemical composition, their atomic density and how the surface planes intercept the bonding network underlying the 3D bulk structure. The resulting surfaces present a complex energy landscape for adsorbates which can act as a template for the growth of 2D crystals with novel structures.

Here we will show new results of 5-fold symmetric molecules which are trapped at 5-fold symmetric sites of the surface, enforcing long-range order in the molecular films (Fig.1). This occurs for  $C_{60}$  molecules on several quasicrystalline substrates [1,2] but also for bowl-shaped corannulene  $C_{20}H_{10}$  molecules on the 5-fold Ag-In-Yb quasicrystalline surfaces. The growth mechanism and the film structure are investigated by STM and LEED complemented by density functional theory calculations. In the case of corannulene molecules with  $C_{5v}$  symmetry, we will discuss their packing strategy when adsorbed on quasiperiodic 5-fold surface compared to 3-fold Pd(111) surface. The growth of quasiperiodic corannulene monolayers on the Ag-In-Yb quasicrystalline surface opens the possibility to achieve 3D-like quasiperiodic molecular films through bowl-in-bowl stacking of the molecules in subsequent deposited layers.



*Fig. 1: From left to right: STM image ( $8 \times 8 \text{ nm}^2$ ) of a  $C_{60}$  film on 10-fold Al-Cu-Co; STM images ( $10 \times 10 \text{ nm}^2$ ) of the clean 5-fold Ag-In-Yb surface ( $10 \times 10 \text{ nm}^2$ ) and after dosing with corannulene ( $8 \times 8 \text{ nm}^2$ ); its corresponding fast Fourier transform and autocorrelation function.*

[1] V. Fournée *et al.*, ACS Nano, 8 (2014) 3646.

[2] J. Smerdon *et al.*, Nano Lett., 14 (2014) 1184–1189.

## Growth of modules on complex Al-based intermetallic compounds: role of order of surface structural complexity

Sam Coates<sup>1</sup>, Abdullah Al-Mahboob<sup>1</sup>, Julian Ledieu<sup>2</sup>, Vincent Fournée<sup>2</sup>, Ronan McGrath<sup>1</sup> and Hem Raj Sharma<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Liverpool, Liverpool L69 3BX, UK*

<sup>2</sup>*Institut Jean Lamour, UMR7198 CNRS, Université de Lorraine, Nancy Cedex, France*

Complex metallic alloy (CMA) surfaces are a fascinating area of materials research due to their outstanding physical properties (brittle nature, high hardness and catalytic activity etc. [1]), indicating promising potential applications. These advantageous properties and, often, the uniqueness of their structural arrangements mean that CMA surfaces have been an intensely researched topic within recent years. The complexity of these alloys is derived from their structure; cluster based formations with 10s, to 1000s of atoms per unit cell – or even an infinite amount in the case of true quasicrystalline (QC) materials [1].

Here, the simple B2-NiAl, the cluster based structure of Al<sub>9</sub>Co<sub>2</sub> and the complex decagonal quasicrystal Al-Ni-Co surface structures have all been studied in an effort to better understand the role that surface geometry takes in molecular adsorption and thin film growth, with zinc-phthalocyanine (ZnPc) and C<sub>60</sub> deposited onto these 3 aluminium based alloys. ZnPc is a member of a family of metal phthalocyanines (MPcs, macrocyclic compounds with metal centres) that have, since their discovery, been used as dyes or pigments [2]. MPcs are an attractive area of research due to their semiconducting properties [2] and, as such, molecular growth in ordered structure is a desirable goal for functionality. The fullerene C<sub>60</sub> molecule has been extensively researched due to its interesting and tuneable electronic properties, which enable them to take a large role in organic electronic devices.

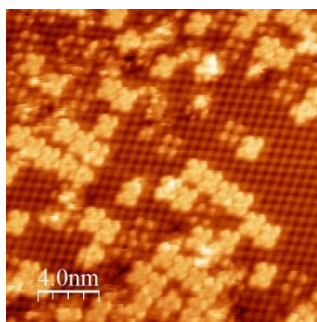


Fig. 1: STM image of low coverage of ZnPc on the Al<sub>9</sub>Co<sub>2</sub> surface

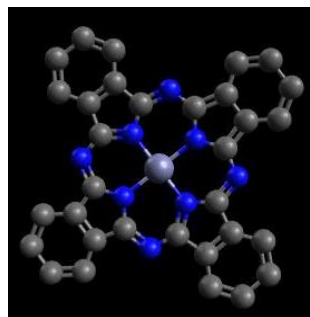


Fig. 2: ZnPc molecule

Using surface sensitive techniques such as scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED), the behaviour of deposited molecules at each surface has been examined with the hope of discovering some long range ordering in the molecular structure, with a view to functionality/application and further understanding of complex surface geometry. ZnPc deposition onto the NiAl(100) surface suggests two preferred adsorption sites, whilst C<sub>60</sub> on the same surface shows no ordering. However, C<sub>60</sub> onto Al-Ni-Co shows QC structure at monolayer coverage, with an ordered structure observed at multilayer growth. ZnPc onto Al<sub>9</sub>Co<sub>2</sub> also appears to exhibit ordered structure (shown in Fig.1), adsorbing to one specific site along a particular direction. Complimentary Density Functional Theory (DFT) calculations will be attempted on the periodic surfaces in order to study adsorption sites and energetics to supplement the physical results.

[1] S. A. Villaseca *et al.*, J. Phys. Chem. C, **115** (30), pp 14922–14932 (2011).

[2] M. Wojdyla *et al.*, Materials Letters, **60** (29-30), pp 3441-3446 (2006).



22<sup>nd</sup> September, Thursday

## **Coverage-dependent structural phase transformations in the adsorption of pentacene on an aperiodically modulated Cu film by DFT**

M. Lahti<sup>1</sup>, K. Pussi<sup>1</sup>, J. A. Smerdon<sup>2</sup>, K. M. Young<sup>3</sup>, H.R. Sharma<sup>3</sup> and R. McGrath<sup>3</sup>

<sup>1</sup>*Lappeenranta University of Technology, School of Engineering Science, P.O. Box 20 FIN-53851 Lappeenranta, Finland.*

<sup>2</sup>*Jeremiah Horrocks Institute for Mathematics, Physics and Astronomy, University of Central Lancashire, Preston PR1 2HE, UK.*

<sup>3</sup>*Surface Science Research Centre, University of Liverpool, Oxford St, Liverpool L69 3BX, UK.*

Surface ordering of pentacene molecules adsorbed on an aperiodic Cu surface has been studied with density functional theory (DFT) as a function of coverage. DFT with vdW functionals is employed to study how the molecule-molecule and molecule-surface interactions evolve as a function of coverage.

Below 0.73 ML, the adsorbate structure is row-like. As the coverage increases the molecules in the row structure get closer together, and the resulting steric effect causes enhanced bending on the molecules. Repulsion between the ends of the molecules forces a chain effect where one end of a molecule bends up and one end of a neighboring molecule bends down. This in turn weakens the molecule-surface interaction. The transition from the row structure to the checkerboard structure takes place at the critical coverage of 0.73 ML ( $5.3 \cdot 10^{13}$  mol cm<sup>-2</sup>). At coverages higher than the critical coverage, a reversion to the row structure is indirectly evidenced via DFT. Raising the number of molecules beyond that which can fit in a checkerboard structure ( $7.1 \cdot 10^{13}$  mol cm<sup>-2</sup>) leads to a close packed row structure as evidenced by STM. DFT simulations are run for coverage of 1.46 ML ( $1.1 \cdot 10^{14}$  mol cm<sup>-2</sup>) which illustrates a situation where all terraces are occupied and on each terrace the Pn molecules are as close as they go. In addition to the bending of the Pn molecules, we also see tilting of the molecules.

## Growth and decay of oxide quasicrystals

Stefan Förster<sup>1</sup>, Jan Ingo Flege<sup>2</sup>, Sebastian Schenk<sup>1</sup>, Eva Maria Zollner<sup>1</sup>, Florian Schumann<sup>1</sup>,  
Rene Hammer<sup>1</sup>, Klaus Meinel<sup>1</sup>, Jens Falta<sup>2</sup>, and Wolf Widdra<sup>1,3</sup>

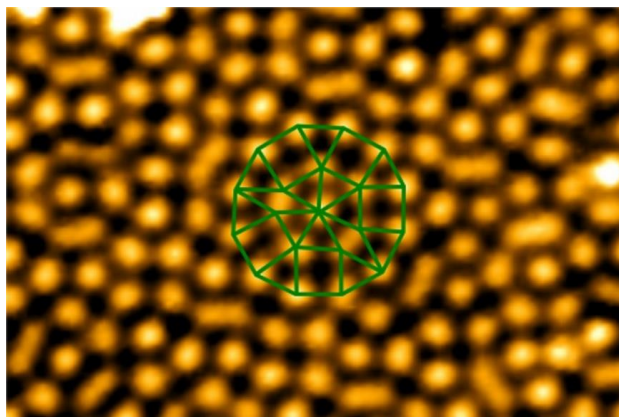
<sup>1</sup>*Martin-Luther-Universität Halle-Wittenberg, Halle, Germany*

<sup>2</sup>*Institute of Solid State Physics, University of Bremen, Bremen, Germany*

<sup>3</sup>*Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany*

A new member in the family of 2D materials is the two-dimensional oxide quasicrystal (OQC) [1]. This OQC develops in a 2D wetting layer spreading from 3D BaTiO<sub>3</sub> islands on Pt(111) and exhibits a sharp twelvefold diffraction pattern [1]. The structure formation process includes the growth of an amorphous wetting layer which can either develop further into the OQC or into long-range ordered periodic structures, the so-called approximants. Insights into this process are derived from combining the findings of scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) measurements with in-situ low-energy electron microscopy (LEEM) studies. Besides the details of the quasicrystalline growth process, the in-situ LEEM studies reveal also the high-temperature stability of this new phase. At temperatures around 900 K, reoxidation in an oxygen atmosphere reconverts the OQC film into 3D BaTiO<sub>3</sub>(111) islands. The observed wetting and dewetting behavior of BaTiO<sub>3</sub> is also found for Ru(0001) and Au(111), although exclusively periodic structures were found here.

Following an analogous preparation procedure, we show that SrTiO<sub>3</sub> on Pt(111) develops an OQC as well. As a consequence of the 2% smaller lattice constant of SrTiO<sub>3</sub> in comparison to BaTiO<sub>3</sub>, the fundamental length of the SrTiO<sub>3</sub>-derived OQC is 2% smaller. Nevertheless, the epitaxial alignment of the SrTiO<sub>3</sub>-derived OQC with respect to Pt(111) is identical to that of the BaTiO<sub>3</sub>-derived OQC. Additionally, both OQCs exhibit the same local atomic arrangement as determined by STM. Our results prove that the interface-driven formation of a 2D OQC is not limited to a particular materials combination.



*Atomically resolved STM image of the Stampfli-Gähler tiling  
of the SrTiO<sub>3</sub>-derived OQC.  $9 \times 6 \text{ nm}^2$ ,  $I = 5 \text{ pA}$ ,  $U = 4 \text{ V}$ .*

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature* 502, 215 (2013).

*This work was supported by the Deutsche Forschungsgemeinschaft (DFG) through the Sonderforschungsbereich SFB 762 “Functional Oxidic Interfaces”.*

## Structural Analysis of Approximants for the BaTiO<sub>3</sub>-derived Oxide Quasicrystal

Martin Trautmann<sup>1</sup>, Florian O. Schumann<sup>1</sup>, Stefan Förster<sup>1</sup>, Sumalay Roy<sup>2</sup>, Rene Hammer<sup>1</sup>, Klaus Meinel<sup>1</sup>, Waheed Adeagbo<sup>1</sup>, Sanjiev K. Nayak<sup>1</sup>, Katayoon Mohseni<sup>2</sup>, Wolfram Hergert<sup>1</sup>, Holger Meyerheim<sup>2</sup>, and Wolf Widdra<sup>1,2</sup>

<sup>1</sup>Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

<sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Recently two-dimensional quasicrystals have been reported which are derived from a transition-metal oxide [1]. For ultrathin films of BaTiO<sub>3</sub> on a Pt(111) single crystal, long-range ordered oxide quasicrystals (OQC) form upon annealing, which show a dodecagonal electron diffraction (LEED) pattern. Scanning tunneling microscopy (STM) reveals a real-space atomic structure that follows the Stampfli-Gähler tiling [2] with self-similar square, triangle, and rhomb arrangements [1].

Here we report the identification of several approximant structures for the dodecagonal OQC: Starting from the same BaTiO<sub>3</sub> ultrathin films on Pt(111), a small modification of the annealing conditions leads to formation of two different long-range ordered approximants.

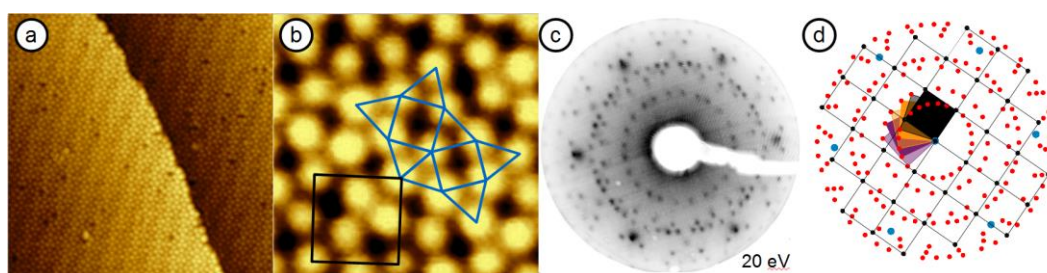


Figure 1: STM (a,b) and LEED (c) of the snub-square approximant to the OQC. Note the six rotational and mirror domains with a nearly quadratic unit cell (black line in (b)) which contribute to the diffraction pattern, schematically shown in (d).

For the approximant with the smallest unit cells known as snub-square (3<sup>2</sup>.4.3.4) tiling, STM shows the atomic structure of the Ti atoms, whereas the LEED data indicate the long-range order (Fig. 1). For a full structure determination, surface x-ray diffraction (SXRD) using synchrotron radiation had been used. On the basis of 44 superlattice reflections, we present the structural model which is consistent with STM and LEED data and is rationalized by DFT calculations. In addition, the phase diagram for existence and coexistence of approximant and quasicrystal structures will be discussed.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature* 502, 215 (2013).

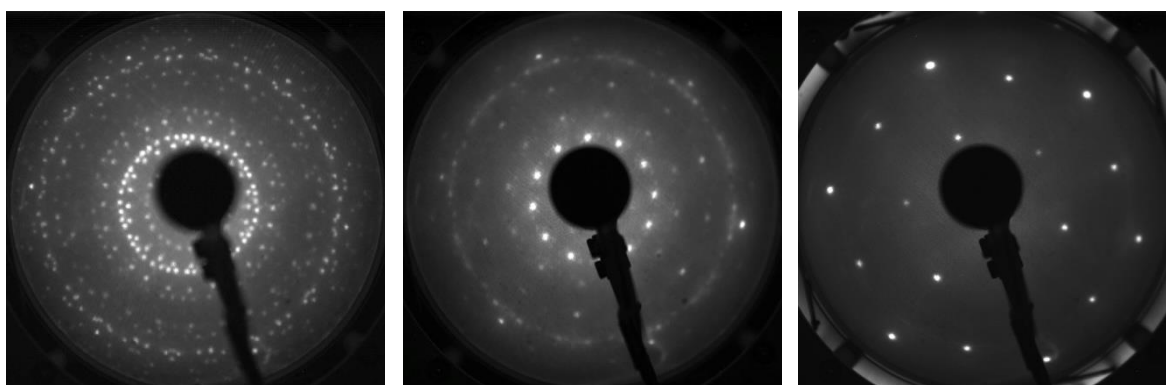
[2] F. Gähler, in *Quasicrystalline Materials*, C. Janot ed. (World Scientific, 1988) p. 272.

## Compositional analysis of oxide quasicrystal : Ba-Ti-O film on Pt(111)

Junji Yuhara, Keito Horiba, and Tokoaki Yamada

*School of Engineering, Nagoya University, Chikusa-ku, Nagoya, 464-8603 Japan*

Recently, as a new family of quasicrystal (QC), metal oxide QC is produced at the Ba-Ti-O film on Pt(111) by Forster [1]. It is very curious to identify the atomic arrangement of Ba, Ti, and O atoms. However, because of the large islands, it has been not easy to examine the surface composition. Structural models are proposed using DFT calculation based on square-triangle-rhomb model [2], since STM shows that the cluster is composed of square-triangle-rhomb. In these models, they assumed the composition to be Ba<sub>0.37</sub>TiO<sub>1.55</sub> for DFT calculations. The purpose of the present study is to prepare island-free QC surface to examine the surface atomic density of Ba, Ti, and O on Pt(111). The sample is prepared by PLD deposition and annealed in UHV or in O atmosphere, otherwise Ti deposition in UHV. The surface is examined by LEED, AES, STM, and XPS. RBS measurements are also performed on Ba-Ti-O films on graphite for calibration curve of XPS intensity and surface atomic density. When the compositional ratio of Ti/Ba is close to 0.5, we could reproduce the quasicrystal surface as well as a crystalline approximant phase and superstructure phase at similar coverages. The LEED patterns observed are displayed in Figure 1. High resolution STM image exhibits exactly the same QC image composed of square, triangle, and rhomb and no islands are observed. From the compositional and chemical analysis using AES, XPS, and RBS, the composition and surface atomic density are proposed.



*Figure 1: LEED patterns of Ba-Ti-O film on Pt(111) with similar compositional ratio  
(a) Crystalline approximant (b) quasicrystal (c) Periodic superstructure*

[1] S. Forster and W. Widdra *et al.*, Nature **502**, 12514 (2012).

[2] E. Cockayne, M. Mihalkovic, C. H. Henley, Phys. Rev. B **93**, 020101 (2016).

22<sup>nd</sup> September, Thursday

## **A complex Self-lubricating, low-friction, wear-resistant Al-based quasicrystalline coatings**

Bruno Alessandro SILVA GUEDES de LIMA,<sup>1,3</sup> Rodinei MEDEIROS GOMES,<sup>1</sup> Severino Jackson GUEDES de LIMA<sup>1</sup>, Diana DRAGOE,<sup>2</sup> Marie-Geneviève BARTHES-LABROUSSE<sup>2</sup>, Richard KOUITAT-NJIWA<sup>3</sup> and Jean-Marie DUBOIS<sup>3</sup>

<sup>1</sup> *Laboratório de Solidificação Rápida, Universidade Federal da Paraíba, João Pessoa-PB, Brazil*

<sup>2</sup> *Institut de Chimie Moléculaire et des Matériaux (UMR 8182 CNRS- Université Paris-Sud 11), Bât. 410, 15 rue Georges Clémenceau , 91405 Orsay Cedex, France.*

<sup>3</sup> *Institut Jean Lamour (UMR 7198 CNRS – Université de Lorraine), Parc de Saurupt, CS50840, 54011 Nancy, France.*

After gas atomization, a quasicrystalline powder based on aluminium is used to prepare a thick coating by high-velocity oxygen-fuel flame torch spraying. This layer is deposited on top of a bond-coat layer on a steel plate. A post-spraying annealing treatment turns the two layers to their stable state, a  $\gamma$ -brass crystal and an icosahedral quasicrystal, respectively. The projection parameters are selected in such a way that the coating behaves like a self-lubricating material, which offers very good wear resistance ( $\lambda$ ) and low friction ( $\mu \leq 6\%$ ), in contrast to the state of the art. This property is achieved thanks to, on the one hand, excellent bonding to the substrate *via* the bond coat, and on the other hand, presence at the boundaries between quasicrystalline flakes of a mixture of both 3-fold and 4-fold coordinated carbon originating from spray processing. Application to hard materials used in mechanical devices is appealing, especially because soft, lubricating additives may not be needed, thus considerably increasing the lifetime of the devices and reducing waste of materials.

22<sup>nd</sup> September, Thursday

## Phason Dynamics in Decagonal Quasicrystals

Hans-Rainer Trebin and Hansjörg Lipp

*Institute for Theoretical and Applied Physics, University of Stuttgart  
Stuttgart, Germany*

In a spectacular experiment of the year 2000, Edagawa et al. observed white spots in HRTEM images of d-AlCuCo, which formed the vertices of a tiling [1]. On a time scale of seconds to minutes the spots changed positions corresponding to phason flips. The questions – only partially answered yet – remain: What is the physical origin of the spots? What is their jump mechanism? Why a time scale in the order of seconds, while atomic jumps occur in picoseconds?

For an answer we employ a structure model of d-AlCuCo which has been proposed by Zeger and Trebin in 1996 [2] as modification of a model of Burkov [3]. It consists of quasiperiodic double layers stacked periodically by 4.18 Å. Each double layer contains rings of ten atoms whose centers form the vertices of a Tübingen triangle tiling. Correlated jumps of two atoms in each sublayer cause a simpleton phason flip of the entire ten ring. The stacking of the double layers leads to columns of the ten rings which might be interrupted due to the flips. Columns which contain a critical minimum number of complete ten rings are visible as white spots.

We postulate microscopic rates for the correlated jumps of the pairs of atoms in the sublayers. The probabilities are calculated for the numbers of complete ten rings in a column, supported by Kinetic Monte Carlo simulations. In this way we find the probabilities that no spot or one spot is visible or that one spot and its flipped copy show up simultaneously. On the basis of these probabilities the mesoscopic time scale for the jumps of the white spots is confirmed.

In our model the ordered initial tiling formed by the white spots is a Tübingen triangle tiling. However, Edagawa et al. [1] and several other authors, for example Ref. [4], observe pentagonal Penrose tilings with much larger density of vertices. We argue, that the observed tilings arise from the triangle tiling due to the simultaneous appearances of vertices and their flipped positions.

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## Diffraction of a simple non-Pisot inflation chain

Michael Baake<sup>1</sup> and Uwe Grimm<sup>2</sup>

<sup>1</sup>*Fakultät für Mathematik, Universität Bielefeld, Postfach 100131, 33501 Bielefeld, Germany*

<sup>2</sup>*School of Mathematics and Statistics, The Open University, Milton Keynes MK7 6AA, UK*

Point sets derived from substitution systems form an important class of aperiodic structures. There are many examples with pure point diffraction, such as the ubiquitous Fibonacci chain and its generalisations, but also paradigms for structures with singular continuous diffraction (the Thue–Morse chain) and absolutely continuous diffraction (the Rudin–Shapiro chain). One can quite easily combine these and produce examples with mixed diffraction spectrum including any combinations of these three components [1].

There is a good understanding of substitutions of constant length, both in one and in higher dimensions [2–4]. Much less is known for non-Pisot substitutions. Here, we concentrate on the primitive two-letter substitution  $a \rightarrow abbb$  and  $b \rightarrow a$  with inflation multiplier  $\lambda = \frac{1+\sqrt{13}}{2}$  as an example. For the one-dimensional point set corresponding to the appropriate geometric realisation in terms of two intervals of length  $\lambda$  and 1, we sketch an argument [5] that indicates that the diffraction, apart from a trivial Bragg peak at the origin, is singular continuous.

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## **Impact of complexity and atomic disorder on lattice dynamics and thermal properties in the complex metallic alloys o-Al<sub>13</sub>Co<sub>4</sub>**

P.-F. Lory<sup>1,2</sup>, V. M. Giordano<sup>3</sup>, P. Gille<sup>4</sup>, M. Mihalkovič<sup>5</sup>, E. Pellegrini<sup>1</sup>, L.-P. Regnault<sup>1</sup>, P. Bastie<sup>1</sup>, H. Schober<sup>1,6</sup>, M. R. Johnson<sup>1</sup>, Y. Grin<sup>7</sup>, M. de Boissieu<sup>2,8</sup>

<sup>1</sup>*Institut Laue-Langevin 71, avenue des Martyrs 38000 Grenoble, France*

<sup>2</sup>*Univ. Grenoble Alpes, SIMAP, F-38000, Grenoble, France*

<sup>3</sup>*ILM, UCBL, CNR, UMR-5586, F-69622, Villeurbanne, Lyon, France*

<sup>4</sup>*Crystallography section Ludwig-Maximilians-Universität München Theresienstrasse 41, 80333 Munich Germany*

<sup>5</sup>*Institute of Physics, Slovak Academy of Sciences 84511 Bratislava, Slovakia*

<sup>6</sup>*Univ. Grenoble Alpes, SIMAP, F-38000, Grenoble, France*

<sup>7</sup>*Max-Planck-Institut für Chemische Physik, fester Stoffe Dresden, Germany*

<sup>8</sup>*CNRS, SIMAP, F-38000, Grenoble, France*

We present a detailed study of the lattice dynamics and its effect on thermal transport property of the Al<sub>13</sub>Co<sub>4</sub> phase which is an approximant to the decagonal AlNiCo phase. This phase, as many other complex metallic alloys displays a low thermal conductivity in the range 1.5 JK<sup>-1</sup>m<sup>-1</sup> [1], whose origin is not yet well understood.

We have performed inelastic neutron and x-ray scattering on a single crystal between 10 and 550K, and compared our results using atomic scale simulation and oscillating pair potentials that are very effective in this system. Whereas along the high symmetry directions we observe phonons whose width is limited by the instrumental resolution, along low symmetry directions we observe a clear signature of a damped harmonic oscillator, for phonon wave vector in the range 3-4 nm<sup>-1</sup>, and a lifetime of the order 2 ps. This lifetime is found to be independent of the temperature, and varies approximately with E<sup>-4</sup>, as expected from phonon scattering on defects. This peculiar behavior, observed for the first time in a CMA, can be reproduced only when the experimentally observed structural disorder has been introduced in molecular dynamic simulations on a 3x2x2 supercell, containing 917 Al and 288 Co atoms. The same model has been used for the simulation of the lattice thermal conductivity that shows weak temperature dependence and compares well with experimental values.

Our results pave the way to a detailed study of phonons and thermal transport properties of a wide range of materials with large unit cell for which local order coexists with structural disorder.

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## Diffuse scattering, phason fluctuations and atomic scale simulation in the Zn-Sc icosahedral quasicrystal

D. Liu<sup>1,2</sup>, T. Yamada<sup>3</sup>, M. Mihalkovič<sup>4</sup>, H. Takakura<sup>5</sup>, M. de Boissieu<sup>1,2</sup>

<sup>1</sup>Univ. Grenoble Alpes, SIMAP, F-38000, Grenoble, France

<sup>2</sup>CNRS, SIMAP, F-38000, Grenoble, France

<sup>3</sup>Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Miyagi 980-9870, Japan

<sup>4</sup>Institute of Physics, Slovak Academy of Sciences 84511 Bratislava, Slovakia

<sup>5</sup>Div. of Applied Physics, Faculty of Engineering, Hokkaido University, Hokkaido 060-8628, Japan,

Understanding the mechanisms that stabilize long range quasiperiodic order remains one of the main challenges in the field. In particular the balance between the energetic and entropic part, in particular the one related to phason fluctuations (see [1]) is far from being understood. Phason fluctuations are known to give rise to a characteristic signature in term of diffuse scattering, which has been observed in all icosahedral quasicrystal, although with a varying intensity and shape anisotropy [1].

We present a detailed study of the binary Zn-Sc quasicrystal, which belongs to the Tsai type quasicrystal [2]. Its structure is described as a packing of three building units: a large triacontahedron (LTR) cluster, a double Friauf polyhedron (DFP) and a prolate rhombohedron [2]. The central part of the cluster is a Zn<sub>4</sub> tetrahedron that induces a strong distortion of the surrounding shells, and breaks their icosahedral symmetry. At high temperature the tetrahedron behaves as a single Zn<sub>4</sub> ‘molecule’ and reorient dynamically with a time scale of the order 1 ps, giving an exceptional dynamical flexibility to this system [3].

A large amount of diffuse scattering is observed in the diffraction pattern, which can be fully accounted for by phason fluctuations with a ratio of the phason elastic constants  $K_2/K_1 = -0.53$ , i.e. close to the 3-fold instability limit.

We will also present atomic scale simulation, using oscillating potentials and large approximant (5/3) for the quasicrystal and large supercell (4x4x4) for the 1/1 approximant. The 5/3 approximant is described as a canonical cell tiling. Molecular dynamics at different temperature has been carried out and the simulated Bragg and diffuse scattering has been followed carefully. Clear differences between the periodic approximant and the quasicrystal have been observed and will be discussed.

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[2] H. Takakura, et al, *Nature Materials* **6** (2007) 58.

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22<sup>nd</sup> September, Thursday

## **Diffraction pattern of quasicrystals with phononic and phasonic disorder – state of art**

Radoslaw Strzalka<sup>1</sup>, Ireneusz Buganski<sup>1</sup>, Maciej Chodyn<sup>1</sup> and Janusz Wolny<sup>1</sup>

<sup>1</sup>*Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland*

Recent development of the statistical approach to structural description of quasicrystals provided a novel method of proper dealing with disorder observed in real structures. Two challenges of modern crystallography of quasicrystals are: (i) including all weak reflections available from diffraction experiments with use of synchrotron radiation, and (ii) how to explain and “repair” the characteristic bias observed in log-log plots of calculated *vs.* measured diffraction intensities during the structure refinement procedure. Modern instruments allow us to collect diffraction datasets of 6 or more orders of magnitude of peak intensities. On the other hand small peaks, which usually have large perpendicular-space component of the scattering vector (see *e.g.* [1] and supplemental materials), are biased in the refinement results. We attribute the latter to the improper corrective factor for phasons, which is standard (exponential) Debye-Waller factor, commonly used in structure refinements of quasicrystals. We perform the credible proofs upon model systems (vertex decoration models) based on Fibonacci chain, Penrose tiling and Ammann tiling.

The statistical approach takes a great advantage of the distribution of atomic positions calculated against some reference lattices [2]. The distribution, called average unit cell and denoted as  $P(u,v)$ , is dense and well defined. It is also highly sensitive to any type of atomic disorder introduced to the structure. Phonons (thermal vibrations of atoms) smear a TAU<sup>2</sup>-scaling  $v=-\tau^2u$  along [1,1]-direction in  $(u,v)$ -space, whereas phasons (rearrangement of atoms [3]) lead to the fragmentation of marginal distribution  $P(u)$ . Both effects are easily noticeable. Knowing the fragmentation of  $P(u)$  we are able to introduce a phasonic corrective factor at the level of structure factor definition (it is not a multiplicative but an additive factor) with one parameter to fit, which is a number of flips in the structure [4].

In the presentation we will explain the basics of our approach and show interesting results of application of the novel Debye-Waller phasonic correction to model systems.

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## **Quasicrystal structure and growth models - a discussion of the status quo and of the still open questions**

Walter Steurer

*Department of Materials, ETH Zurich, 8093 Zurich, Switzerland*

There are approximately one hundred stable decagonal and icosahedral quasicrystals known so far in binary and ternary intermetallic systems. What do we know about their structures? How far do we understand the principles of their formation and growth? What is the essence in this regard of the more than 12 000 publications on quasicrystals that appeared so far? I will shortly sketch the progress in the development of the models for the growth of quasicrystals as well as for their structures. I will also address the strengths and limits of these models, and point out where improvements may be necessary and feasible. One of the questions is whether the state of the art in quasicrystal research is already comparable to that in complex intermetallics in general. Another question is, what we could learn from the studies on mesoscopic quasicrystals for the structure formation of intermetallic quasicrystals. Or, a very basic question, what exactly do we have to know and to prove experimentally before we can say we fully understand the formation of quasicrystalline order.

## Magnetic Properties of Icosahedral Quasicrystals

Alan I. Goldman<sup>1,2</sup>

<sup>1</sup>*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

<sup>2</sup>*Ames Laboratory, US DOE, Iowa State University, Ames, Iowa 50011, USA*

In the thirty-five years since the discovery of quasicrystals by Dan Shechtman there has been tremendous progress in our understanding of the structure of quasicrystals, and we have recently seen a surge of activity and new results regarding the electronic, magnetic, optical and thermal properties of these systems. The discoveries of a new family of magnetic quasicrystals<sup>1</sup>, exhibiting spin-glass-like behavior<sup>2</sup>, and their closely related crystalline approximants<sup>3</sup> which manifest long-range magnetic order at low temperature, offer new opportunities for studies of the impact of aperiodicity on magnetic interactions in compounds that have similar local structures. Here, I will focus on progress in our understanding of magnetism in quasicrystals and their related periodic approximants,<sup>4</sup> with an eye to future investigations that can shed further light on the role of aperiodicity in shaping physical properties.

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## **Perspectives in quasicrystal research: the mathematics of quasicrystals**

Antoine Julien

*Institutt for matematiske fag, Norwegian university of science and technology,  
7491 Trondheim, Norway, e-mail: antoine.julien@math.ntnu.no*

Central to crystallography is the notion of symmetry. The very discovery of quasicrystals was prompted by a diffraction pattern with a “forbidden” five-fold symmetry. The corresponding mathematical question (“which relevant objects stay the same when acted upon by a group?”) is far from obvious: what are the objects, what are the groups, and what does it mean to stay the same?

In this talk, I will present some of the objects which were introduced to deal with quasicrystals (namely the hull and the algebra), and explain a few mathematical questions related to these objects. I will also highlight new interactions of the mathematical theory of aperiodic order with group theory, number theory, and signal analysis.

## Phase transitions toward complex electronic states and superperiodic structures in monophosphate tungsten bronzes

Olivier Pérez

*Laboratoire CRISMAT, UMR 6508 CNRS, ENSICAEN 6 Boulevard du Marechal Juin, 14050 Caen CEDEX 4, France*

Monophosphate tungsten bronzes (MPTB) with the chemical formula  $(\text{PO}_2)_4(\text{WO}_3)_{2m}$  and  $m$  ranging from 2 to 14 can be described by the regular stacking of  $\text{PO}_4$  tetrahedra slices and  $\text{WO}_6$  octahedra slabs<sup>1</sup>; the thickness of the tungsten slab is proportional to  $m$ . MPTB are quasi 2D metals and show quasi-2D electronic character due to 5d conduction electrons confined with  $\text{WO}_6$  layers. They exhibit successive phase transitions toward charge density wave (CDW) states at different critical temperatures  $T_{p1}$ ,  $T_{p2}$  ... These transitions are associated to lattice distortions leading to the appearance of incommensurate or commensurate structural modulations. This family of compounds, with the electronic dimensionality governed by the  $m$  parameter, is thus a relevant system to analyze the influence of the dimensionality on the electronic instabilities such as CDW states.

CDW transitions exhibit signature both from structural and physical properties point of view; X-ray diffraction experiments using classical sources but also synchrotron radiations as well as physical properties analysis (transport, magnetism ...) can be then used to characterized electronic instabilities.

Accurate studies of the phase transitions were performed for MPTB with different  $m$  values using X-ray thermo diffraction as well as transport measurements. High resolution structural studies and novel experimental techniques will be described. Structural analysis in the fundamental but also in the CDW states using synchrotron radiation is proposed. These complementary investigations evidenced different characteristics for members with low or high  $m$  values such as symmetry lowering; incommensurate or commensurate modulations; first order or second order phase transition ... All these new results will be presented and compared with results previously reported<sup>3,4,5,6</sup>.

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## Bioactivity of quasicrystalline-reinforced composite materials for 3D printing of medical implants

Guillaume Cini<sup>1</sup>, Thibaud Chatel<sup>1</sup>, David Bonina<sup>1</sup>, Olivier Godard<sup>1</sup>, Aude Falanga<sup>2</sup>, Vincent Fournée<sup>1</sup>, Samuel Kenzari<sup>1</sup> and Nguyen Tran<sup>2</sup>

<sup>1</sup>*Institut Jean Lamour, UMR 7198 CNRS – Université de Lorraine, Nancy, FRANCE*

<sup>2</sup>*Défaillance Cardiovasculaire Aiguë et Chronique, UMR S 1116 INSERM – Université de Lorraine, Vandoeuvre-lès-Nancy, FRANCE*

Biocompatible polymer materials are known since several decades in tissue engineering and in particular for their use as medical implants. However, despite their mechanical properties being comparable to that of human cortical bone, some polymers suffer from being bioinert. To tackle this problem, numerous studies have been focused on the development of polymer-based composite materials, by adding bioactive particles into the polymer matrix.

Earlier work found that polymer-quasicrystal composites are biocompatible [1]. More recent studies showed that such composites can be processed by 3D printing technologies to produce parts with improved functional properties [2]. Additive manufacturing of materials with improved bioactive properties in the medical field could be extremely promising for bone regeneration. In this context, we will show that quasicrystalline-reinforced polymer composites do not only present improved mechanical properties but also exhibit very high bioactivity as assessed by a cell test (Figure 1) compared to other reference composites. This work opens new opportunities for medical applications of quasicrystalline alloys.

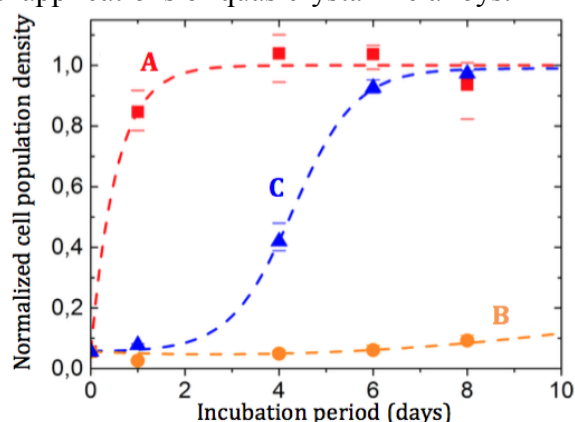


Figure 1: Comparison of the evolution of cell population density for a polymer-quasicrystal composite (A), the polymer matrix (B) and a non-cytotoxic reference (C).

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## The microstructure and hydrophobic behavior of Al-Cu-Fe coating by plasma spraying

Tai-Sheng Chen, Wu-Han Liu and Ming-Sheng Leu<sup>1</sup>

<sup>1</sup>*Materials and Chemical Laboratory (MCL), Industrial Technology Research Institute (ITRI), Hsinchu 31040, Taiwan. No.195, ChungHsing Road, Sec. 4, Hsinchu 31040, TAIWAN;*

The quasicrystalline (QC) materials has been reported in 1984 by Shechtman et al [1]., it have become the subject of intense study due to their crystallographically forbidden fivefold symmetry axis, therefore possess unique properties, such as high resistivity, low thermal conductivity, high hardness, wear resistance, low friction coefficient, anti-corrosion, oxidation resistance and hydrophobic compared with traditional metal material. However, the mechanical properties of quasicrystal materials are similar to those of intermetallic compounds, it is very hard but low toughness in bulk at ambient temperature, therefore not proposed applications employ quasicrystalline coating by magnetron sputtering and thermal spraying. Moreover, thermal spraying is more suitable for industrialized quasicrystalline coating production. The purpose of this study was to prepare and evaluate the microstructure and hydrophobic behavior of Al-Cu-Fe coating by using plasma spraying. The structural, morphology, chemical composition, mechanical property and hydrophobic behavior of coating were characterized by alpha-stepper profiler, Grazing Incidence X-ray Diffraction (GIXRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), Vicker's indentation and contact angle measurement, respectively. The surface morphology of Al-Cu-Fe coating by SEM was shown in the Fig. 1 (a). The ~200 nm nanoparticle were formed of nanostructured Al-Cu-Fe coating after 800°C annealing result in increasing the hydrophobic behavior. The contact angle of nanostructured Al-Cu-Fe coating after 800°C annealing was shown in the Fig. 1 (b). The contact angle Al-Cu-Fe coating after 800°C annealing is about 135°, it's better than convention Al-Cu-Fe and PTFE coating (~110°) due to nanoparticle formation on the surface of Al-Cu-Fe coating. The hardness of Al-Cu-Fe coating were reached over ~Hv 700. The relationship between the process, microstructure and hydrophobic behavior of Al-Cu-Fe coating was discussed and established.

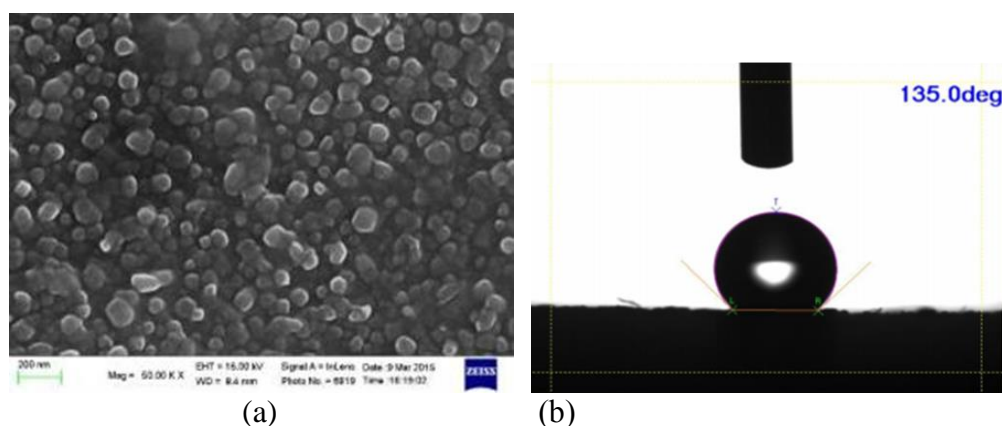


Figure 1: (a) The surface morphology and (b) contact angle of Al-Cu-Fe coatings after 800 °C annealing. .

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## **Mechanical properties of carbon nano-variant reinforced quasicrystal composite**

T. P. Yadav<sup>1</sup>, D. Singh<sup>1,2</sup>, M. A. Shaz<sup>1</sup>, N. K. Mukhopadhyay<sup>3</sup>, R. K. Mandal<sup>3</sup> and O. N. Srivastava<sup>1</sup>

<sup>1</sup>*Hydrogen Energy Centre, Department of Physics, Banaras Hindu University, Varanasi-221005, India*

<sup>2</sup>*Departement of Physics, Panjab University, Chandigarh 160014, India*

<sup>3</sup>*Department of Metallurgical Engineering, Indian Institute of Technology (BHU), Varanasi-221 005, India*

Intermetallics based nano-composite materials are of great importance, because they exhibit higher fracture toughness and strength than the conventional intermetallics including quasicrystals [1]. In this work, nano-composite materials have been developed using Al<sub>65</sub>Cu<sub>20</sub>Fe<sub>15</sub> icosahedral quasicrystal as the matrix and different form of the carbon nano-variants as reinforcement's i.e. mechanically activated carbon (graphite), carbon nano-tube, carbon nano-fiber and graphene individually. The mechanically activated carbon was prepared using a high-energy planetary mill at 600 rpm in toluene medium as a process control agent within 80 h and other carbon nano-variants i.e. carbon nano-tube, carbon nano-fiber and graphene have been prepared by chemical vapor deposition technique at different physical conditions. The composite materials were prepared using locally fabricated low intensity ball mill (up to 100 rpm) where carbon nano-variants were homogenously mixed/ dissolved into quasicrystalline matrix. Mechanical behavior of the compressed and sintered samples (at 200 °C) showed an increase in the hardness as well as fracture toughness of the quasicrystal-carbon nano-tube composite materials up to 20 at%. The high hardness value may be attributed to the different microstructure resulting due to the addition of different carbon nano-variants. The details structural and microstructure of four different composite materials in the context of the hardness will be addressed during the conference.

Keywords: Carbon, Composite, Quasicrystal, Mechanical activation, Hardness, fracture toughness.

[1] T.P. Yadav et al. Materials Letters 80 (2012) 5–8

23<sup>rd</sup> September, Friday

## **Characteristic smearing wear behavior of quasicrystals as abrasive materials**

Yongjun Chen, Jianbin Qiang, Chuang Dong

*Key Lab of Materials Modification by Laser, Ion, and Electron Beams (Ministry of Education), School of Materials Science and Engineering, Dalian University of Technology, Dalian 116024, China*

The quasicrystalline structure and its unique mechanical response characteristics [1] give rise to potential applications as soft metal abrasive materials [2]. The abrasive polishing behavior of  $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$  quasicrystal on soft metal such as Cu and stainless steel alloys were investigated, to compare with commonly used hard abrasives including diamond, alumina and silica. A unique surface flaw repairing effect has been discovered in the experiments, and a smearing-type wear mechanism is proposed to explain the phenomenon, in sharp contrast to all the other three abrasives. Such an effect is the direct result of severe surface plastic deformation upon polishing using quasicrystal abrasives following the characteristic smearing-type polishing mechanism.

Key word: Quasicrystals abrasive; Polishing; Smearing-type mechanism.

23<sup>rd</sup> September, Friday

## **American physical society publications and peer review process in PRB**

Hari Dahal

*American Physical Society*

“The American Physical Society (APS) is a non-profit membership organization working to advance and diffuse the knowledge of physics through its outstanding research journals, scientific meetings, and education, outreach, advocacy, and international activities”(aps.org). APS publishes leading scientific journals including Reviews of Modern Physics, Physical Review Letters, Physics (online only) and The Physical Review, which cover a broad area of physics research. The Physical Review comprises of a series of journals such as Physical Review A, B, C, D, E, X, and Applied. Physical Review B (PRB) is the largest and most comprehensive international journal covering the subject of condensed matter and materials physics. In this presentation, I will mostly talk about the mechanism of peer review process in PRB.

## List of Poster Presentations

Poster No	Presenter	Title
P01	Jean-Marie Dubois	Partial densities of states in binary Al-based intermetallics
P02	Y. Sekiyama	Electron localization and conduction mechanism of icosahedral quasicrystal Al-Pd-Ru
P03	Nobuhisa Fujita	Atomic structure of the primitive cubic phase P40 in the Al-Pd-Ru system
P04	T. Onodera	Structural vacancy density in icosahedral quasicrystal Al <sub>170.7</sub> Pd <sub>21.34</sub> Re <sub>7.96</sub>
P05	Lax Chan	Inflation-based sequences with absolutely continuous spectrum
P06	Dvir Flom	"Color" code for the brick tiling
P07	Shuya Matsukawa	Magnetic properties of the Au-Al-Yb approximant under hydrostatic pressure
P08	Ma. Lailani B. Walo	Color groups of colorings of N-planar Modules
P09	N. Ito	Synthesis and magnetic properties of the Au-Al-Yb approximant
P10	Y. Tanaka	Synthesis of Au-Ga-Yb quasicrystal
P11	Libor Ďuriška	Thermodynamic description of $\epsilon$ -area in the Al-Pd system
P12	Ivona Černičková	Atomic structure of epsilon phase
P13	H Parsamehr	Effect of annealing time on the mechanical and surface properties of Al-Cu-Fe quasicrystal thin films
P14	Marek Adamech	Experimental study of phases I and H in selected (56-60)Zn-(29-35)Mg-(8-13)Y alloys after long-term annealing at 400°C
P15	Thakur P. Yadav	Structural stability of decagonal phase in Al-Ga-Pd-Mn alloy
P16	Hiroyuki Takakura	Cluster environments in a twelve-fold packing model of icosahedral quasicrystals
P17	Dmitriy Shulyatev	Electron transport in Al-Cu-Co-Fe quasicrystals and approximants
P18	A. Ishikawa	Magnetic properties of rare-earth containing Tsai-type approximants
P19	R. Maeda	Thermoelectric properties of Al <sub>63</sub> Cu <sub>25</sub> Fe <sub>12-x</sub> (Au,Pt) <sub>x</sub> quasicrystals
P20	Kotoba Toyonaga	Formation conditions of dodecagonal quasicrystal in Mn-Cr-Ni-Si alloys
P21	Rei Sasaki	Synthesis and electronic properties of the Au-Sn-Yb approximant
P22	Tomonari Dotera	Origin of 18-fold quasicrystal
P23	Kazue Nishimoto	TEM observations of superlattice structure in Al <sub>2.75</sub> Ir and Al <sub>2.63</sub> Rh 1/0 approximants

P24	An Pang Tsai	Interfacial stability for quasicrystals-dispersed Mg alloys in Mg-Cd-Yb system
P25	Joe Smerdon	Templated Quasicrystalline Molecular Layers
P26	Tsunetomo Yamada	Icosahedral quasicrystal and approximant phases in Au-(Ga, Si, Sn)-Yb alloy systems
P27	Masahiko Shimoda	Hard x-ray photoelectron spectroscopy (HAXPES) studies on quasicrystals and approximant crystals
P28	K. Yamada	Evaluation of structural defects using positron annihilation study for 1/1-AlReSi approximant crystals made by spark plasma sintering
P29	Kazuki Nozawa	Adsorption structure of Bi on the fivefold surface of i-Ag-In-Yb quasicrystal
P30	Akira Yoshiasa	Crystalline approximants in the Al-rich part of the Al-Ru-Ni System
P31	Yoshitaka Matsushita	Reinvestigation of 'Dy <sub>5</sub> Pd <sub>2</sub> ', crystal structure of Dy <sub>71.17</sub> Pd <sub>24.48</sub> (~Dy <sub>5.81</sub> Pd <sub>2</sub> )
P32	Hem Raj Sharma	Thin film growth in quasicrystal surfaces
P33	Lokendra Poudel	Metal ions, solvent effects, hydrogen bonding, electronic structure and topology in G-quadruplex DNA
P34	Samir Paudel	Magnetism in zigzag and armchair CuO nanotubes: ab-initio study
P35	Narayan P Adhikarai	First-Principles study of a molecular adsorption of water on MoS <sub>2</sub> /Graphene bilayer hetero-structures
P36	Saran Lamichhane	Electronic structures and concentration dependent magnetism on NiGa and Ni <sub>3</sub> Ga
P37	Bishnu Prasad Paudel	First-principles study of electronic and magnetic properties of manganese decorated graphene
P38	Maryam Kiani	The comparison of magnetic and physical properties of quasicrystals with their constituting elements
P39	Maryam Kiani	Study of deposition method of the each Al, Pd elements on the Al-Pd-Mn Quasicrystal

# **Abstracts For Poster Presentations**

## Partial Densities of States in binary Al-based intermetallics

Esther BELIN-FERRÉ<sup>1</sup>, Guy TRAMBLY de LAISSARDIÈRE<sup>2</sup> and Jean-Marie DUBOIS<sup>3</sup>

<sup>1</sup> *LCPMR (Sorbonnes Université, Université Pierre et Marie Curie, UMR 7614), 11 rue P. et M. Curie, F-75231 Paris cedex 5.*

<sup>2</sup> *Laboratoire de Physique Théorique et Modélisation (LPTM - UMR 8089) Université de Cergy-Pontoise / CNRS, 2 avenue Adolphe Chauvin, F-95302 Cergy-Pontoise Cedex.*

<sup>3</sup> *Institut Jean Lamour (UMR 7198 CNRS – Université de Lorraine), Parc de Saurupt, CS50840, 54011 Nancy, France.*

We account in this paper for a two-decade long study of the partial densities of states in periodic Al-TM (TM: transition metal) binary compounds the compositions of which are reminiscent of those of quasicrystals found in ternary systems like Al-Cu-Fe or Al-Ni-Co. The study is based, on the one hand, on experimental data derived from soft X-ray emission spectroscopy at both the edges of Al and of TM, and on the other hand, on computations issued from *ab initio* methods. Special attention is placed on the pseudo-gap at the Fermi energy and its influence on stabilizing a specific structure as well as on hybridization between Al and the TM constituent. A correlation is pointed out between depth of the pseudo-gap and complexity of the crystalline lattice. Reference is made to information already published for quasiperiodic materials of comparable composition.

## Electron localization and conduction mechanism of icosahedral quasicrystal Al-Pd-Ru

Y. Sekiyama<sup>1</sup> and I. Kanazawa<sup>1</sup>

<sup>1</sup>*Department of Physics, Tokyo Gakugei University, 4-1-1, Nukuikitamachi, Koganei, Tokyo 184-8501, Japan*

One of the most outstanding properties of quasicrystals is the electrical conductivity above and below the metal-insulator transition [1].

One of the present authors [2-4] has considered the transport property in the randomly distributed system of the correlated configuration is  $\sim 2\pi/2k_F$  (the quasicrystal-like state).

The quasicrystal-like state is regarded as the system composed of the Gaussian correlated distribution of the icosahedral cluster, while includes  $2k_F$ -phase shift scattering.

Taking into account the short mean free path, 15-20 Å of the electrons in quasicrystals, the transport property in the quasicrystal-like system might be closely analogous to the one in the quasicrystal system.

In this study, by comparing with experimental data [5], we shall consider the electronic transport property in quasicrystal Al-Pd-Ru, taking into account the conduction mechanism in the quasicrystal-like system.

[1] S.J.Poon, *Adv. Phys.* **41**, 303(1992)

[2] I.Kanazawa, *Physica. E* **18**, 306 (2003)

[3] T.Akiyama, Y.Takagiwa, I.Kanazawa, *Philos. Mag.* **86**, 747(2006)

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[5] R.Tamura *et al.*, *J.Phys. Condens. Matter.* **11**, 10343(1999)



## Atomic structure of the primitive cubic phase $P_{40}$ in the Al-Pd-Ru system

Yusuke Hatakeyama, Nobuhisa Fujita and An Pang Tsai

*Institute of Multidisciplinary Research for Advanced Materials,  
Tohoku University, Sendai 980-8577, Japan*

In the Al-Pd-Ru phase diagram, there exist an icosahedral quasicrystal and a few kinds of cubic crystalline approximants [1]. Among others, the  $P_{40}$  phase attracts our interest because of the large unit-cell size (lattice constant  $\approx 40\text{\AA}$ ) and hence of its proximity to icosahedral quasicrystallinity. There has been no report on the atomic structure of  $P_{40}$  due primarily to the difficulty in synthesizing a fine single crystal grain for X-ray studies, whereas electron diffraction patterns (e.g. in [1]) suggest that the crystal structure may be similar to that of the primitive cubic approximant in the Al-Pd-Cr-Fe system reported recently [2]. The aim of the present study is to elucidate the atomic structure of the  $P_{40}$  phase in Al-Pd-Ru.

After an ingot with the reported composition  $\text{Al}_{72.6}\text{Pd}_{13}\text{Ru}_{14.4}$  for  $P_{40}$  [1] was annealed at  $1000^\circ\text{C}$  for 480 hours, a single crystal grain 3mm in diameter wrapped in a polycrystalline domain was obtained. The composition of the grain was analyzed with ICP to be  $\text{Al}_{72}\text{Pd}_{16.4}\text{Ru}_{11.6}$ , which deviates from that of the whole ingot. Still, powder X-ray diffraction indicated that the crystal was  $P_{40}$ , then a single crystal X-ray diffraction measurement was performed. The software package JANA2006 [3] was used to analyze the crystal structure.

The determined crystal structure is shown in Fig. It comprises two kinds of clusters with some minor disorders. The  $P_{40}$  phase in Al-Pd-Ru turns out to be isostructural to the Al-Pd-Cr-Fe approximant [2], which is characterized as a  $2\times 2\times 2$  superstructure of the  $3/2$ -cubic approximant. The results will be presented in more detail at the ICQ13.

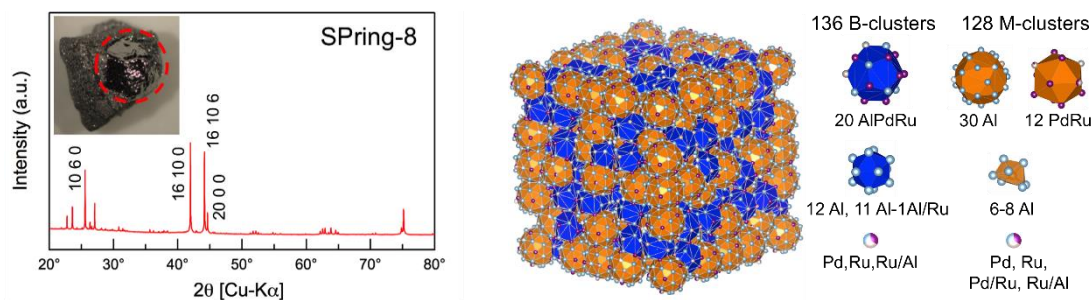


Figure 1: (left) Single grain and its powder XRD pattern.  
(right) Crystal structure of the  $P_{40}$  phase in Al-Pd-Ru.

[1] D. Pavlyuchkov *et al.*, J. Alloys Comp. **469**, 146 (2009). [2] N. Fujita, *et al.*, Acta Cryst. **A69**, 322 (2013). [3] V. Patricek *et al.*, JANA2006: <http://jana.fzu.cz/> (2006).

## Structural Vacancy Density in icosahedral quasicrystal $\text{Al}_{70.7}\text{Pd}_{21.34}\text{Re}_{7.96}$

T. Onodera, Y. Sekiyama, I. Kanazawa, M. Matsumoto

*Department of Physics, Tokyo Gakugei University, Koganeshi, Tokyo 184-8501, Japan*

It has been suggested that the stability of quasicrystals might be derived from Hume-Rothery rule. In addition, it has been argued that whether cluster centers are vacant or occupied by an atom is important in the electronic states and the thermal stability of quasicrystal [1]. According to the molecular orbital calculation, an Al-12 icosahedron cluster without center atom shows more covalent bonding, whereas an Al-13 icosahedron cluster with center atom has more metallic one[2]. Furthermore Yamada et al. [3] have discussed the relationship between structured vacancies and anomalous transport properties of stable Al-based quasicrystals. In this study, we have estimated the structural vacancy density of the icosahedral quasicrystal  $\text{Al}_{70.7}\text{Pd}_{21.34}\text{Re}_{7.96}$  by means of statistical diffusion method for thermalized positrons, taking into account the structural model for  $\alpha$ -phase Al-Mn-Si.

[1] K. Kimura et al, J.Solid.State.Chem. **133**, 302 (1997)

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## Inflation-based sequences with absolutely continuous spectrum

Lax Chan and Uwe Grimm

*School of Mathematics and Statistics, The Open University, Milton Keynes MK7 6AA, UK*

The Rudin-Shapiro sequence [1,2] is the paradigm for a substitution-based structure with (in the balanced weight case) purely absolutely continuous diffraction spectrum; see [3] for details and background. It shares this property with balanced weight random sequences (almost certainly in the probabilistic sense), so sequences with absolutely continuous spectrum are, as such, not uncommon. However, not many examples of substitution-based systems are known. In [4], it is shown that Hadamard matrices give rise to substitution systems in one or more dimensions with vanishing pair correlation functions. More generally, the results of [5,6] imply that, at least in the constant length substitution case, the substitution-based system needs to have vanishing pair correlation in order to show absolutely continuous diffraction. Intuitively, the reason behind this is that any non-vanishing correlation at a given distance gives rise to correlations at larger distances due to the self-similar structure of the substitution system, and hence gives rise to singular diffraction.

In this work, we start from Rudin's original approach [2], and modify it in order to obtain further examples of substitution-based sequences with absolutely continuous diffraction. The simplest new example employs a four-letter substitution of length four, and is investigated in more detail, using Bartlett's approach [6].

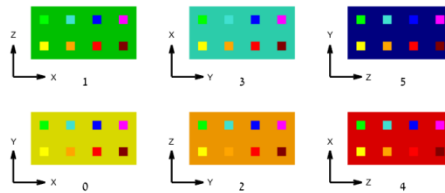
- [1] H.S. Shapiro, *Extremal Properties for Polynomials and Power Series*, Masters thesis (MIT, Boston, 1951).
- [2] W. Rudin, Some theorems on Fourier coefficients, *Proc. Amer. Math. Soc.* **10**, 855-859 (1959).
- [3] M. Baake, U. Grimm, *Aperiodic Order. Volume 1: A Mathematical Invitation* (Cambridge University Press, Cambridge, 2013).
- [4] N.P. Frank, Substitution sequences in  $\mathbb{Z}^d$  with a non-simple Lebesgue component in the spectrum, *Ergod. Th. & Dyn. Syst.* **23**, 519-532 (2003).
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## "Color" code for the brick tiling

Dvir Flom and Shelomo I. Ben-Abraham

*Department of Physics, Ben-Gurion University, IL-8410501 Beer Sheba, Israel*

We have constructed a three-dimensional analog of the two-dimensional table tiling [1] – a *brick tiling*. Here we show generations 0 through 4 of the tiling. Here we also present its corresponding lattice substitution tiling. It is based on a "color" code that faithfully labels every basic cube of the tiling. Its prototiles are, in turn,  $d!2^{(d-1)d/2} = 3!2^{2 \times 3/2} = 3!2^3 = 6 \times 8 = 48$  basic cubes (henceforth called "protobricks"). They are labeled by numbers 0 through 5 and six colors; the basic cubes in each protobrick are labeled by numbers 0 through 7 and eight colors as shown in Figure 1. Thus the code has entries of two digits and/or two colors. In an arbitrary dimension  $d \in \mathbb{N}$  a brick has edges  $2^0, \dots, 2^{d-1}$  and consists of  $2^{(d-1)d/2}$  basic cubes. It comes in  $d!$  orientations. While in 2D this seems to be dual to the chair tiling in any higher dimension the two tilings are very different. The numbers relating to the brick tiling rapidly become staggering.



*Figure 1: The colors of the six protobricks.*

[1] E. A. Robinson Jr., *Indag. Mathem. N.S.* **10**, 581 (1999).

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## Magnetic Properties of the Au-Al-Yb approximant under hydrostatic pressure

Shuya Matsukawa<sup>1</sup>, Kazuhiko Deguchi<sup>1</sup>, Keiichiro Imura<sup>1</sup>, Tsutomu Ishimasa<sup>2</sup>, and Noriaki K. Sato<sup>1</sup>

<sup>1</sup>*Department of Physics, Nagoya University, Nagoya, 464-8602, Japan*

<sup>2</sup>*Division of Applied Physics, Hokkaido University, Sapporo, 060-8628, Japan*

Quantum criticality has been considered to be specific to crystalline materials such as heavy fermions, until the Tsai-type quasicrystal  $\text{Au}_{51}\text{Al}_{34}\text{Yb}_{15}$  was reported to show unusual quantum critical behavior, i.e., the divergent feature of the magnetic susceptibility and the electronic specific heat coefficient with an unusual critical index as  $T \rightarrow 0$  [1]. In addition, the robustness of the quantum criticality of the quasicrystal against the application of hydrostatic pressure is also unusual. On the other hand, the Au-Al-Yb approximant does not show such the diverging behavior at ambient pressure. Recently, we observed that the magnetic susceptibility of the approximant at  $P_c \simeq 2$  GPa diverges with the same critical index as the quasicrystal [2]. At high pressures greater than  $P_c$ , we found that the magnetic state emerges at low temperatures. However, it is not clear yet whether this is a long-range ordered state or a spin-glass-like short-range ordered state.

Figure 1 shows the temperature dependence of the nonlinear susceptibility,  $\chi_2$ , of the approximant at 2.79 GPa. We observe an anomaly at  $T \simeq 0.1$  K, the temperature where the ac susceptibility shows the cusp like anomaly. This result is interpreted as indicating that the magnetic phase is a spin-glass-like short-range ordered state. At the conference, we will present the experimental results of the conventional and nonlinear susceptibilities under pressure.

[1] K. Deguchi, S. Matsukawa, N. K. Sato, T. Hattori, K. Ishida, H. Takakura and T. Ishimasa, *Nat. Mater.* **11**, 1013 (2012).

[2] S. Matsukawa, K. Deguchi, K. Imura, T. Ishimasa and N. K. Sato, submitted to *J. Phys. Soc. Jpn.*

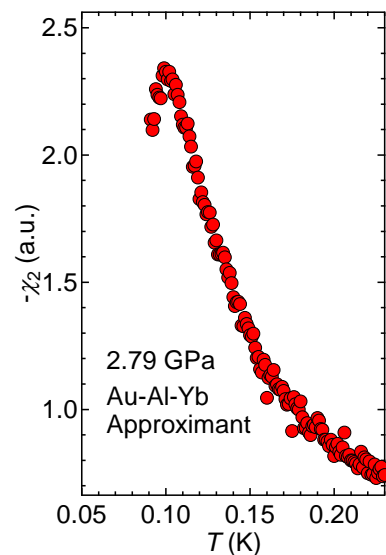


Fig.1. Temperature dependence of the nonlinear susceptibility of the Au-Al-Yb approximant at 2.79 GPa.

## Color groups of colorings of $N$ -planar modules

Manuel Joseph C. Loquias, Lilibeth D. Valdez and Ma. Lailani B. Walo

*Institute of Mathematics, College of Science, University of the Philippines-Diliman  
Diliman, 1101 Quezon City, Philippines*

A submodule of a  $\mathbf{Z}$ -module determines a coloring of the module where each coset of the submodule is associated to a unique color. Given a submodule coloring of a  $\mathbf{Z}$ -module, the group formed by the symmetries of the module that induces a permutation of colors is referred to as the color group of the coloring. In this presentation, a method to solve for the color groups of colorings of plane  $N$ -modules where  $N=4$  and  $N=6$ , that is, when the  $N$ -module is a lattice, is given. An example involving a coloring of the Ammann-Beenker tiling is given to exhibit how these methods may be extended to the general case.

- [1] M. Baake, *Combinatorial aspects of colour symmetries*, J. Phys. **A30** (1997), no. 8, 2687-2698.
- [2] E. P. C. Bugarin, M.L.A.N. De Las Penas, and D. Frettlöh, *Perfect colourings of cyclotomic integers*, Geom. Dedicata(2013) **162**, 271-282 .
- [3] M.L.A.N. De Las Penas and R.P. Felix, *Color groups associated with square and hexagonal lattices*, Z. Krist. **222** (2007), no. 10, 505-512.

## Synthesis and magnetic properties of the Au-Al-Yb approximant

N. Ito<sup>1</sup>, A. Ishikawa<sup>1</sup>, T. Hiroto<sup>2</sup>, K. Tokiwa<sup>3</sup>, T. Watanuki<sup>4</sup> and R. Tamura<sup>1</sup>

<sup>1</sup>*Department of Materials Science and Technology, Tokyo University of Science, Tokyo 125-8585Japan*

<sup>2</sup>*Graduate School of Frontier Sciences, The University of Tokyo, Chiba 77-8561Japan*

<sup>3</sup>*Department of Applied Electronics, Tokyo University of Science, Tokyo 125-8585Japan*

<sup>4</sup>*Condensed Matter Science Division, Quantum Beam Science Directorate, Japan Atomic Energy Agency, Hyogo 679-5148Japan*

Various phenomena such as a quantum critical state and superconductivity have been observed in Tsai-type intermediate valence quasicrystals and approximants [1] [2]. In these compounds, the Yb valence can be varied by applying the pressure [3] [4]. However, so far, there has been no report on the composition dependence of intermediate valence in these systems. Recently, it has been reported that the Au-Al-Gd approximant has a wide single phase region accompanying a systematic change of the magnetism [5]. In the present work, we have investigated the single phase region of the Au-Al-Yb approximant and studied the composition dependence of the Yb valence. Polycrystalline alloys of nominal compositions of Au<sub>x</sub>Al<sub>86-x</sub>Yb<sub>14</sub> (x = 52-64) were prepared by arc-melting high-purity (>99.9 wt%) Au, Al, Yb. The alloys were annealed under an Ar atmosphere. The phase purity of the samples was examined by powder X-ray diffraction using Cu K $\alpha$  radiation. The temperature and field dependence of the magnetization were measured using SQUID and VSM in the temperature range between 1.8 K and 300 K and fields of up to 9 T. The Yb valence of the Au-Al-Yb approximant at room temperature were measured by Yb L<sub>3</sub>-edge x-ray absorption near-edge structure (XANES) spectroscopy in BL22XU at SPring-8. Powder X-ray diffraction studies have shown that a single phase is obtained in a wide Au/Al range with 14 at% Yb. The lattice parameter is found to increase drastically within a specific composition range. The temperature dependence of magnetic susceptibility is found to be strongly dependent on the composition, suggesting the change of the Yb valence in the Au-Al-Yb approximant. Details of the magnetic measurements will be presented in the poster.

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[2] K. Deguchi, *et al.*, J. Phys. Soc. Jpn. **84**, 023705 (2015)

[3] D. Kawana, *et al.*, Phys. Rev B **81**, 220202(R) (2010).

[4] T. Watanuki, *et al.*, Phys. Rev B **86**, 094201 (2012).

[5] A. Ishikawa, *et al.*, Phys. Rev B **93**, 024416 (2016).

## Synthesis of Au-Ga-Yb quasicrystal

Y. Tanaka<sup>1</sup>, T. Seki<sup>2</sup>, N. Shibata<sup>2</sup>, T. Fujii<sup>3</sup>, R. Tamura<sup>1</sup>

<sup>1</sup>*Department of Materials Science and Technology, Tokyo University of Science,  
Tokyo 125-8585 Japan*

<sup>2</sup>*Department of Materials Science & Engineering, University of Tokyo, Tokyo 113-8656  
Japan*

<sup>3</sup>*Cryogenic Research Center, the University of Tokyo, Tokyo 113-0032 Japan*

In 2011, the icosahedral Au-Al-Yb quasicrystal was discovered[1], which was found to be intermediate valence state at ambient pressure[2]. Also, In 2015, it was reported that Au-Ge-Yb 1/1 cubic approximant has superconductivity[3]. From these things, Au-based quasicrystal/approximant has attracted particular interest from various aspects. In the Au-Ga-Yb system, no quasicrystals has been reported and we searched for a new quasicrystal in this ternary system.

Polycrystalline alloys of various in the Au-Ga-Yb system were prepared by arc-melting high-purity Au, Ga, Yb. The phase purity of the samples was examined by powder X-ray diffraction using CuK $\alpha$  radiation and also by TEM observation. The temperature and field dependence of the magnetization were measured using a SQUID magnetometer in the temperature range between 1.8 and 300 K and fields of up to 1000 Oe. The temperature of the electrical resistivity were measured using a PPMS in the temperature range between 0.5 and 300 K.

As a result of the search, we have found a new icosahedral quasicrystal in the Au-Ga-Yb system. Magnetic susceptibility and electrical resistivity will presented in the poster.

[1]T. Watanuki, *et al.*, *Phys. Rev. B* **86**, (2012) 176-183.

[2]K. Deguchi, *et al.*, *Nature materials*, **11**, (2012) 1013-1016.

[3]K. Deguchi, *et al.*, *J. Phys. Soc. Jpn.* **84**, 023705 (2015).



## Thermodynamic description of $\varepsilon_n$ -area in the Al-Pd system

Libor Ďuriška<sup>1</sup>, Ivona Černíčková<sup>1</sup>, Roman Čička<sup>1</sup>, Pavol Priputen<sup>1</sup>, Dušan Janičkovič<sup>2</sup>, Jozef Janovec<sup>3</sup>

<sup>1</sup>*Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, Paulínska 16, 917 24 Trnava, Slovak Republic*

<sup>2</sup>*Institute of Physics, Slovak Academy of Sciences, Dúbravská 9, 845 11 Bratislava, Slovak Republic*

<sup>3</sup>*Slovak University of Technology in Bratislava, Vazovova 5, 812 43 Bratislava, Slovak Republic*

The Al-Pd system has been thermodynamically assessed by Li et al. [1]. Despite of a good coincidence between both calculated [1] and experimental phase diagrams [2], several differences around the Al<sub>3</sub>Pd composition are evident. The non-stoichiometric  $\varepsilon_n$  area, occurring in the experimental phase diagram, is described by stoichiometric phases Al<sub>3</sub>Pd and Al<sub>21</sub>Pd<sub>8</sub> in the calculated diagram. The aim of this work is to describe Al<sub>3</sub>Pd, calculated as stoichiometric up to now, as a non-stoichiometric  $\varepsilon_n$  by means of the CALPHAD method. As a result, the area of occurrence of the non-stoichiometric  $\varepsilon_n$  around the Al<sub>3</sub>Pd stoichiometry was involved in the calculated Al-Pd phase diagram. The (Al%,Pd)<sub>3</sub>(Al,Pd%)<sub>1</sub> two-sublattice thermodynamic model was used to describe  $\varepsilon_n$ , marked as (Al<sub>3</sub>Pd) in the thermodynamic notation. A novel thermodynamic description of the (Al<sub>3</sub>Pd) phase was obtained. Existing thermodynamic parameters of stoichiometric phases Al<sub>4</sub>Pd and Al<sub>21</sub>Pd<sub>8</sub> were slightly adjusted due to involving the thermodynamic model of non-stoichiometric (Al<sub>3</sub>Pd). To verify the results of thermodynamic calculations, alloys Al<sub>72.4</sub>Pd<sub>27.6</sub> and Al<sub>67</sub>Pd<sub>33</sub> were experimentally investigated. In the Al<sub>67</sub>Pd<sub>33</sub> alloy annealed at 500°C, the eutectoid reaction,  $\varepsilon_n \leftrightarrow \text{Al}_{21}\text{Pd}_8 + \text{Al}_3\text{Pd}_2$ , at around 625°C was proved.

[1] M. Li, Ch. Li, F. Wang, and W. Zhang, *Intermetallics* **14**, 39 (2006).

[2] B. Grushko, *J. Alloys Comp.* **557**, 102 (2013).

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## Atomic structure of epsilon phase

Ivona Černičková<sup>1</sup>, Libor Ďuriška<sup>1</sup>, Ľubomír Čaplovič<sup>1</sup>, Marek Mihalkovič<sup>2</sup>, Pavol Priputen<sup>1</sup>,  
Jozef Janovec<sup>3</sup>

<sup>1</sup>*Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology  
in Trnava, Paulínska 16, 917 24 Trnava, Slovak Republic*

<sup>2</sup>*Institute of Physics, Slovak Academy of Sciences, Dúbravská 9, 845 11 Bratislava,  
Slovak Republic*

<sup>3</sup>*Slovak University of Technology in Bratislava, Vazovova 5, 812 43 Bratislava,  
Slovak Republic*

In this work, several phases of the  $\varepsilon$ -family (denoted jointly as  $\varepsilon_n$  [1,2]) were studied in more detail. Phases of the  $\varepsilon$ -family are classified as orthorhombic approximants of the decagonal quasicrystal [3]. In the Al-Pd-Co system,  $\varepsilon_6$  and  $\varepsilon_{28}$  were classified as binary phases alloyed with the third element, and  $\varepsilon_{16}$ ,  $\varepsilon_{22}$  and  $\varepsilon_{34}$  as ternary phases [1].

Alloys Al<sub>73</sub>Pd<sub>27</sub>, Al<sub>74</sub>Pd<sub>26</sub>, Al<sub>70</sub>Pd<sub>25</sub>Co<sub>5</sub>, Al<sub>71.2</sub>Pd<sub>15</sub>Co<sub>13.8</sub>, Al<sub>72.5</sub>Pd<sub>21</sub>Co<sub>6.5</sub>, Al<sub>72.8</sub>Pd<sub>15.6</sub>Co<sub>11.6</sub>, Al<sub>73.3</sub>Pd<sub>12.8</sub>Co<sub>13.9</sub>, Al<sub>76</sub>Pd<sub>11</sub>Co<sub>13</sub> were investigated after annealing at 850°C for 500 h, 700°C for 2000h or 700°C for 500h. In the investigation, scanning electron microscopy including energy dispersive X-ray spectroscopy, X-ray diffraction, transmission electron microscopy, and scanning transmission electron microscopy using high-angle annular dark-field detector were used. Based on experimental results, phason models and cluster arrangements of  $\varepsilon_6$ ,  $\varepsilon_{16}$  and  $\varepsilon_{28}$  phases were proposed. The attention was also paid on the comparison of experimentally determined and modelled structures. The structural model of the orthorhombic  $\varepsilon_n$  based on pseudo-Mackay icosahedra and large bicapped pentagonal prism clusters was confirmed experimentally.

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## **Effect of annealing time on the mechanical and surface properties of Al-Cu-Fe quasicrystal thin films**

H. Parsamehr, Shou-Yi Chang, Chih-Huang Lai

Department of Material science and Engineering, National Tsing Hua University, Hsinchu, 30013, Taiwan.

**Abstract.** Quasicrystals are known for their unique mechanical properties. Previous research has shown that these properties can be optimized during fabrication. The annealing process is one way to produce quasicrystal thin films with optimized mechanical properties. Temperature during annealing has been shown to affect mechanical properties; however annealing time has not yet been considered. Here, three AlCuFe samples were sputtered on Si/SiO<sub>2</sub> substrates in a three-step process. Samples were then annealed in a two-step process for different durations (5, 10 and 15 hours). Additionally, one non-quasicrystal AlCuFe thin film was produced to emphasize the importance of the composition. X-ray Diffraction (XRD) data showed a sharper quasicrystal peak for the sample annealed for 15 hours. From nano indentation measurements, we saw that the 15-hour annealed sample had the greatest hardness. Also the sample annealed for the longest duration had a higher contact angle. This work shows that annealing time, like temperature, has an effect on the I-phases, and thus on the mechanical properties of quasicrystals.

**Keywords-** Quasicrystal; AlCuFe; Annealing time; Mechanical properties; Thin film

## Experimental study of phases I and H in selected (56-60)Zn-(29-35)Mg-(8-13)Y alloys after long-term annealing at 400°C

Marek Adamech<sup>1</sup>, Ivona Černíčková<sup>1</sup>, Ľubomír Čaplovič<sup>1</sup>, Pavol Priputen<sup>1</sup>, Dušan Janičkovič<sup>2</sup>, Jozef Janovec<sup>3</sup>

<sup>1</sup> Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, Paulínska 16, 917 24 Trnava, Slovakia

<sup>2</sup> Slovak Academy of Sciences, Institute of Physics, Dúbravská 9, 845 11 Bratislava, Slovakia

<sup>3</sup> Slovak University of Technology in Bratislava, Vazovova 5, 812 43 Bratislava, Slovakia

Even if Zn-Mg-Y alloys have been studied sporadically since ninetieths years of the last century [1-5], the obtained findings do not facilitate to any exhaustive description of this system. Based on experimental results, Tsai et al. [1] proposed partial isothermal sections of the Zn-Mg-Y phase diagram at temperatures 427°C, 500°C and 600°C, containing homogeneity ranges of ternary phases Z, W, H and I. The calculated isothermal sections of this diagram at 600°C, 500°C and 400°C were reported by Grobner et al. [5].

A lack of experimental and calculated data related to the (I+H) area evoked the current study. Five (56-60)Zn-(29-35)Mg-(8-13)Y alloys (metal compositions are given in at.%) were investigated after annealing at 400°C for 150 h. In the investigation, the scanning electron microscopy including energy dispersive X-ray spectroscopy and the X-ray diffraction were used. The alloys were selected with the intention to collect experimental data about the (I+H) phase equilibrium at 400°C and to show trends applicable in a refinement of the related isothermal section of the Zn-Mg-Y phase diagram. As a result, a specific isothermal section at 400°C of Zn-Mg-Y phase diagram was presented, showing both own experimental results and related thermodynamic and experimental results available in literature.

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## Structural stability of decagonal phase in Al-Ga-Pd-Mn alloy

T.P. Yadav<sup>1</sup>, Devinder Singh<sup>1,2</sup>, R.R. Shahi<sup>1,3</sup>, M.A. Shaz<sup>1</sup>, N.K. Mukhopadhyay<sup>4</sup>,  
R.S. Tiwari<sup>1</sup>, and O.N. Srivastava<sup>1</sup>

<sup>1</sup>*Department of Physics, Banaras Hindu University, Varanasi 221005, India*

<sup>2</sup>*Departement of Physics, Panjab University, Chandigarh 160014, India*

<sup>3</sup>*Department of Physics, Motilal Nehru National Institute of Technology,  
Allahabad, 211004, India*

<sup>4</sup>*Department of Metallurgical Engineering, Indian Institute of Technology (BHU),  
Varanasi 221005, India*

The effect of Al substitution by Ga on the microstructure and the stability of decagonal quasicrystalline phase in  $\text{Al}_{70-x}\text{Ga}_x\text{Pd}_{13}\text{Mn}_{17}$  alloys has been studied as shown in the previous papers [1]. The as-cast and rapidly solidified alloys with  $x = 0, 2.5$  and  $5$  have been investigated and it was shown that the alloys up to  $5$  at.% Ga exhibit the formation of small amount of icosahedral quasicrystalline phases along with major amount of decagonal phase in the rapidly solidified ribbons. In the present investigation, the structural stability up to  $20$  at.% Ga with respect to thermal treatments of the  $\text{Al}_{70-x}\text{Ga}_x\text{Pd}_{13}\text{Mn}_{17}$  decagonal phase has been explored. Both in the as-cast and rapidly solidified condition, the decagonal phases up to  $10$  at % Ga have been observed. The as-cast alloys were annealed at  $800$  °C for  $72$  h while the rapidly solidified ribbons were annealed at  $600$  °C for  $72$  h. The alloys have been characterized by X-ray diffraction, scanning & transmission electron microscopy, energy dispersive x-ray analysis and differential thermal analysis techniques. Characteristic features of these alloys will be discussed with reference to their structural microstructural evolution.

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## Cluster Environments in a Twelve-fold Packing Model of Icosahedral Quasicrystals

Hiroyuki Takakura<sup>1</sup> and Radoslaw Strzalka<sup>2</sup>

<sup>1</sup>*Division of Applied Physics, Faculty of Engineering Hokkaido University, Sapporo, Hokkaido, 060-8628, Japan*

<sup>2</sup>*Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland*

A successful structural description for icosahedral quasicrystals (iQCs) is now available as the Yb-Cd iQC model in which Tsai-type clusters are arranged at the twelve-fold packing sites, a subset of the vertices of Ammann-Kramer-Neri (AKN) tiling [1-4]. Possible cluster connections are those along 2- and 3-fold directions (so-called *b*- and *c*-links), and those along 5-fold directions, *a*-links, are excluded. Therefore the six-dimensional model is constructed based on the occupation domain having a specific shape for the twelve-fold packing sites (Fig.1(a)). The twelve-fold packing sites have coordination numbers in the range from 7 to 12 [2, 3, 5]. Frequencies for 18 different cluster environments were calculated numerically for this specific occupation domain [5]. The aim of this work is to present the exact shapes of the occupation domains for each cluster environment (Fig.1(b)). This information would be useful when one consider an extended model including local chemistry for ternary iQCs or a similar model with different cluster types, such as Bergman or Mackay types.

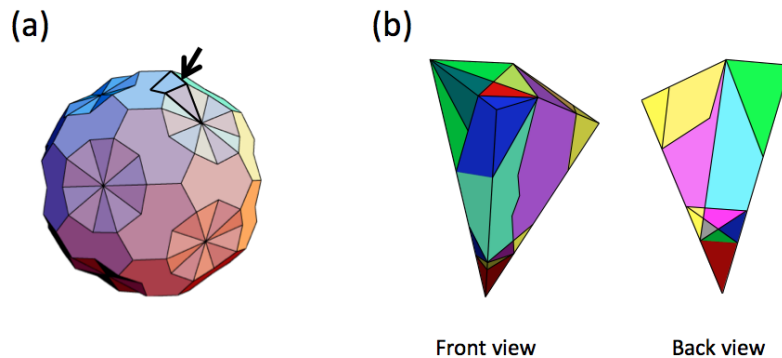


Figure 1: (a) The archetype occupation domain for the 12-fold packing sites, and (b) its asymmetric unit (arrowed part in (a)), colored with respect to each cluster environment.

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## Electron Transport in Al–Cu–Co–Fe Quasicrystals and Approximants

Dmitriy Shulyatev<sup>1</sup>, Maria Klyueva<sup>1</sup>, Nikolay Andreev<sup>1</sup>, Tatiana Sviridova<sup>1</sup>, Natalia Tabachkova<sup>1</sup> and Alexey Suslov<sup>2</sup>

<sup>1</sup>*National University of Science and Technology MISiS, Moscow, 119049, Russian Federation*

<sup>2</sup>*National High Magnetic Field Laboratory, Tallahassee FL, 32310, USA*

A huge number of studies have been carried out to investigate the influence of a crystal structure on physical properties of icosahedral and decagonal quasicrystals and their crystalline approximants which consist of the same atomic clusters. The quaternary Al–Cu–Co–Fe system presents a special interest from this point of view because it contains both decagonal and icosahedral phases and their approximants.

To study anisotropy of electron transport in Al–Cu–Co–Fe quasicrystals and approximants a row of Al–Cu–(Co,Fe) single crystals (with linear sizes of a few millimeters) with a different Co/Fe ratio have been grown by the slow cooling of a quaternary melt. Phase and chemical composition as well as crystal structure of the obtained single crystals have been studied by XRD, EDX, SAED and back-Laue analysis. The crystal structure of the Al–Cu–(Co,Fe) single crystals continuously changed with decreasing Co/Fe ratio from 2D aperiodic decagonal quasicrystalline through orthorhombic decagonal approximant to monoclinic icosahedral approximant (Fig.1). Temperature dependences of resistivity and magnetoresistance in the obtained single crystals have been investigated. The electron transport of quasicrystals and approximants is discussed in relation to their crystal structure.



*Figure 1: icosahedral approximant Al<sub>65</sub>Cu<sub>18</sub>Co<sub>7</sub>Fe<sub>10</sub>: single crystal (a) and SAED parents along the threefold (b) and twofold (c) zone axes.*

## Magnetic properties of rare-earth containing Tsai-type approximants

A. Ishikawa<sup>1</sup>, T. Hiroto<sup>2</sup>, K. Tokiwa<sup>3</sup>, T. Fujii<sup>4</sup>, T. Takeuchi<sup>5</sup>, and R. Tamura<sup>1</sup>

<sup>1</sup>*Department of Materials Science and Technology, Tokyo University of Science, Tokyo (Japan)*

<sup>2</sup>*Graduate School of Frontier Sciences, The University of Tokyo, Chiba (Japan)*

<sup>3</sup>*Department of Applied Electronics, Tokyo University of Science, Tokyo (Japan)*

<sup>4</sup>*Cryogenic Research Center, The University of Tokyo, Tokyo (Japan)*

<sup>5</sup>*Department of Technology, Toyota Technological Institute, Aichi (Japan)*

The behavior of spins in quasiperiodic structure is one of the fundamental issues in the physics of quasicrystals (QCs) and their approximants (ACs). Rare-earth containing Tsai-type QCs and ACs have been investigated since they have well-localized spin on the icosahedron shell. Recently, the existence extensively of a long-range magnetic order was reported in Cd<sub>6</sub>Tb and Au-SM-R (SM = Si, Ge, Sn) Tsai-type ACs [1-3]. Therefore, it has now become of great interest to investigate the magnetic properties of other Tsai-type compounds that are also composed of the same Tsai-type clusters. In the present work, we have studied the phase constitution and magnetic properties in the Au-Al-Gd systems [4].

Polycrystalline alloys were prepared by arc-melting and annealed under Ar atmosphere. The phase purity of the samples was examined by powder X-ray diffraction (XRD) using CuK $\alpha$  radiation. The temperature and field dependence of the magnetization were measured using a SQUID or VSM magnetometer. The specific heat was measured using MPMS or PPMS.

Powder X-ray diffraction studies have shown that Au-Al-Gd possesses an extraordinary wide single-phase region with 14 at% Gd. Also, the lattice parameter is found to increase with increasing the Au/Al ratio. Magnetic measurements have shown a salient composition-driven spin-glass to ferromagnetic transition in the approximant crystal for the first time. An interesting feature of Au-Al-Gd is that the paramagnetic Curie temperature,  $\Theta_p$ , is clearly dependent on the Au/Al ratio.  $\Theta_p$  increases significantly from a large negative value to a large positive value as the Au content increases. The behavior of  $\Theta_p$  is explained based on the RKKY oscillation. Detailed results of the magnetic properties will be reported in the presentation.

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## Thermoelectric properties of $\text{Al}_{63}\text{Cu}_{25}\text{Fe}_{12-x}(\text{Au,Pt})_x$ quasicrystals

R. Maeda<sup>1</sup>, Y. Takagiwa<sup>2</sup>, I. Kanazawa<sup>1</sup>, K. Kimura<sup>3</sup>, S. Ohhashi<sup>4</sup>, and A. P. Tsai<sup>4</sup>

<sup>1</sup>*Department of Physics, Tokyo Gakugei University, Tokyo 184-8501, Japan*

<sup>2</sup>*National Institute for Materials Science (NIMS), Ibaraki 305-0047, Japan*

<sup>3</sup>*Department of Advanced Materials Science, the University of Tokyo, Chiba 277-8561, Japan*

<sup>4</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577, Japan*

Al-based icosahedral quasicrystals are attractive for thermoelectric (TE) applications because of the formation of pseudogap near the Fermi level,  $E_F$ , and their complexity in structures, which simultaneously lead to a large power factor and a low lattice thermal conductivity [1]. For practical TE applications, materials should be low cost and non-toxic, possessing high TE performance. Therefore, we selected thermodynamically stable Al-Cu-Fe quasicrystal for tuning the thermoelectric properties.

There are few reports on the high-temperature thermoelectric properties of Al-Cu-Fe system. Bilušić *et al.* reported the electrical conductivity, Seebeck coefficient, Hall coefficient, and thermal conductivity of  $\text{Al}_{62}\text{Cu}_{25.5}\text{Fe}_{12.5}$  and  $\text{Al}_{63}\text{Cu}_{25}\text{Fe}_{12}$  from 4.2 K to 340 K [2,3]. The sign of the Seebeck coefficient depends on the sample composition, *i.e.* the position of  $E_F$  in the electronic density of states, indicating that both *p*- and *n*-type materials can be obtained in the same alloy system. As expected from the complex crystal structure, the low thermal conductivity of 2–5 W/m·K at 300 K has been found in Al-Cu-Fe quasicrystal. However, it is still necessary to lower the phonon thermal conductivity for improving TE figure of merit,  $zT$ . We discuss herein the alloying effect through Au and Pt substitutions for Fe on the phonon thermal conductivity of  $\text{Al}_{63}\text{Cu}_{25}\text{Fe}_{12-x}(\text{Au,Pt})_x$  ( $x = 0, 1, 2, 3$ ) quasicrystals. We expected that Pt and Au atoms behave as a scattering center in the matrix. Also, we will present the data of the Seebeck coefficient and the electrical conductivity up to 873 K.

The dense bulk samples were synthesized by arc-melting, annealing, followed by spark plasma sintering. The resulting bulk density distributed 4.5–4.9 g/cm<sup>3</sup> with varying  $x$ , which was high enough to assess the thermoelectric properties at high temperatures.

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## Formation conditions of dodecagonal quasicrystal in Mn-Cr-Ni-Si alloys

Kotoba Toyonaga, Shuhei Iwami and Tsutomu Ishimasa

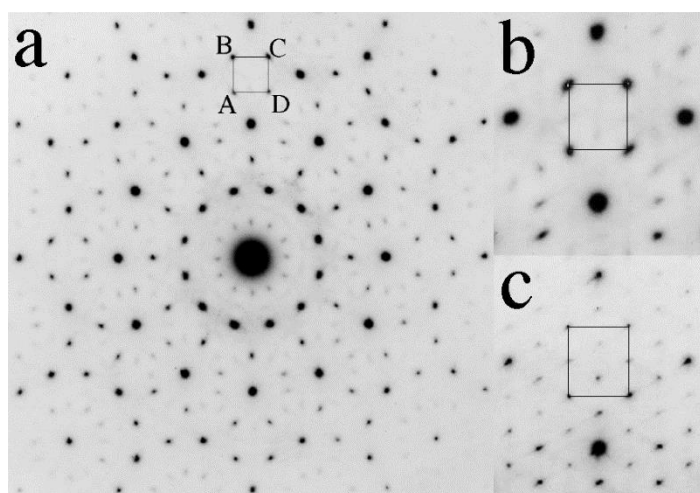
Graduate School of Engineering, Hokkaido University, Kita-ku, 060-8628 Sapporo, Japan

In this study, the formation conditions of the dodecagonal quasicrystal, which forms in the Mn-Cr-Ni-Si system [1], have been studied in order to improve its structural quality. The as-cast specimens with the composition  $\text{Mn}_{72.0}\text{Cr}_{15.5}\text{Ni}_{15.0}\text{Si}_{17.5}$  were prepared by arc melting. They were heated to various temperatures in the range of 600-1024 °C with heating rate 1-3 K/min, and held at the temperature for various periods from 15 to 320 h. The specimens were studied by means of X-ray diffraction technique and selected-area electron diffraction method using an aperture corresponding to 2500 Å in diameter.

We describe here experimental results on the specimens annealed at 600 °C. All the specimens include the dodecagonal quasicrystal besides the dominant  $\beta$ -Mn type structure. An electron diffraction pattern of the quasicrystal is presented in Fig. 1a. In this pattern the arrangement of reflections satisfies the 12-fold symmetry, and all the reflections are indexed by the following formula with four indices  $h_n$  ( $a = 4.560$  Å).

$$\mathbf{g}_{//} = \sum_{n=1}^4 h_n \mathbf{a}_n^*, \quad \mathbf{a}_n^* = \frac{1}{\sqrt{3}a} \left[ i \cos \frac{(n-1)\rho}{6} + j \sin \frac{(n-1)\rho}{6} \right] \quad \text{for } n = 1 \sim 4,$$

In the ideal case, the quadrangle indicated by thin lines in Fig. 1a is a square, of which four vertices are A:  $\bar{2}0320$ , B:  $\bar{2}0330$ , C:  $\bar{1}0330$  and D:  $\bar{1}0320$  reflections. Therefore the shape of the quadrangle can be a measure of the quality of the quasicrystal. In the case of the hexagonal approximant ( $a_h = 17.03$  Å,  $c_h = 4.630$  Å) shown in Fig. 1c, the quadrangle is a rectangle with the ratio of two edges:  $\xi = 2/\sqrt{3} = 1.155$ . The ratio  $\xi$  is 1.02(1) in Fig. 1a indicating that the quality of the quasicrystal is high. However, the pattern with larger ratio ( $\xi = 1.08$  (2)) was also



observed (Fig. 1b). Such low-quality regions frequently coexist in the present specimens.

Figure 1: Electron diffraction patterns. Notice that patterns in (b) and (c) are slightly magnified.

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## Synthesis and electronic properties of the Au-Sn-Yb approximant

R. Sasaki<sup>1</sup>, T. Hiroto<sup>2</sup>, T. Fujii<sup>3</sup> and R. Tamura<sup>1</sup>

<sup>1</sup>*Department of Materials Science and Technology, Tokyo University of Science, Tokyo 125-8585 Japan*

<sup>2</sup>*Graduate School of Frontier Sciences, The University of Tokyo, Chiba 277-8561 Japan*

<sup>3</sup>*Cryogenic Research Center, The University of Tokyo, Tokyo 113-0032 Japan*

Recently, various electrical properties have been reported in some Yb-bearing Tsai-type quasicrystals and their 1/1 approximants. For example, the first observation of superconductivity in quasicrystal-related materials was reported in the Au-Ge-Yb 1/1 approximant [1], and also much attention has been paid to a quantum critical state of the Au-Al-Yb quasicrystal [2]. On the other hand, there are few reports about physical properties of approximants with higher order than 1/1 approximants. Therefore, it is of great interest to investigate the electrical properties of Yb-bearing Tsai-type 2/1 approximants such as, for example, Au-Sn-Yb system [3]. In the present work, we have investigated the single phase region and studied the electrical properties of the Au-Sn-Yb 2/1 approximant.

Polycrystalline Au-Sn-Yb alloys of various nominal compositions were prepared by arc-melting high-purity (>99.9 wt%) Au, Sn and Yb. The alloys were annealed at 773 K under an Ar atmosphere. The phase purity of the samples was examined by powder X-ray diffraction (XRD) using CuK $\alpha$  radiation and the composition was examined by fluorescent X-ray spectroscopy (XRF). The temperature dependence of the electrical resistivity was measured by the four-probe method in the temperature range between 0.5 and 300 K.

The XRD and XRF studies showed that the single phase region of the 2/1 approximant is extended within a range of 2 at% for each element. Two different behaviors were observed in the temperature dependence of the electrical resistivity. One group exhibits a negative temperature coefficient of electrical resistivity below 300 K. Another exhibits a positive temperature coefficient between 150 K and 300 K, and a negative coefficient below 100 K. The behavior seems to be dependent on the Au and Yb concentrations. Detailed results including other properties will be reported in the presentation.

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## Origin of 18-fold quasicrystal

Shinichi Bekku<sup>1</sup>, Primož Ziherl<sup>2,3</sup>, and Tomonari Dotera<sup>1</sup>

<sup>1</sup>*Department of Physics, Kindai University, 3-4-1 Kowakae, Higashi-Osaka 577-8502, Japan*

<sup>2</sup>*Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia*

<sup>3</sup>*Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia*

Since soft quasicrystals were discovered in nature, a new research front has emerged in the field of quasicrystals [1]. In particular, Fischer *et al.* found that colloidal micelles in solution self-assembled into a 18-fold quasicrystalline phase [2], whose symmetry has not been found in synthetic metallic compounds. They used PI<sub>30</sub>-PEO<sub>120</sub> block copolymers based on the hydrophobic polyisoprene (PI) and the hydrophilic polyethylene oxide (PEO). In aqueous solution, these block copolymers self-assembled into spherical core-shell micelles where the well-defined core of PI blocks is surrounded by a thick shell of PEO blocks. Presently, the real-space structure of quasicrystals formed by these micelles is still unknown.

To investigate 18-fold quasicrystals theoretically, we have numerically explored a 2D system of disks with a purely repulsive hard-core/square-shoulder pair interaction and found a high-density phase of 18-fold symmetry [3]. With a large fraction of particles forming close-packed equilateral triangles, the phase is structurally similar to the dodecagonal quasicrystalline phase except that the four-sided tiles that it contains are rhombi rather than squares. In this presentation, we study the structure of the 18-fold phase in more detail, focusing on the mechanisms of its formation by examining the development of the bond-orientational order parameters at low temperatures. We find that the so-called special clusters of particles play a crucial role in the mixing of the three sets of bond directions 20° apart, producing the 18-fold diffraction pattern.

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## TEM observations of superlattice structure in $\text{Al}_{2.75}\text{Ir}$ and $\text{Al}_{2.63}\text{Rh}$ 1/0 approximants

K. Nishimoto<sup>1</sup>, N. Yamaguchi<sup>2</sup>, R. Tamura<sup>2</sup>, M. Terauchi<sup>1</sup>, A.P. Tsai<sup>1</sup>

<sup>1</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577 Japan*

<sup>2</sup>*Department of Materials Science and Technology, Tokyo University of Science, Tokyo, 125-8585 Japan*

The structure of Al-TM(TM=Ir, Rh) 1/0 quasicrystalline approximants ( $\text{Al}_{2.75}\text{Ir}$  and  $\text{Al}_{2.63}\text{Rh}$ ) were reported a primitive cubic lattice with the space group P23 or Pm3[1]. The unit cell consist of pseudo-Mackay icosahedral cluster and there is a TM atom in centre of the TM icosahedron. Interestingly, the Al-TM 1/0 approximants possesses disordered 9~10 Al inside of the TM icosahedron. Recently, we observed very weak superlattice spots in the selected area electron diffraction patterns for binary  $\text{Al}_{2.75}\text{Ir}$  [2]. Additionally, the order-disorder phase transition of Al inside TM icosahedron is predicted by pair potentials fitted to an ab initio database [2]. In this work, we report that TEM study of the superstructure and electronic structures of the  $\text{Al}_{2.75}\text{Ir}$  and  $\text{Al}_{2.63}\text{Rh}$  1/0 approximants.

Figure 1 shows selected area electron diffraction patterns of (a) $\text{Al}_{72.5}\text{Rh}_{27.5}$  and (b) $\text{Al}_{74.5}\text{Rh}_{25.5}$ . We observed the superlattice spots in the case of Al-rich composition. The composition dependence on the superstructure suggests that the number of Al inside the TM icosahedron contribute to the superstructure.

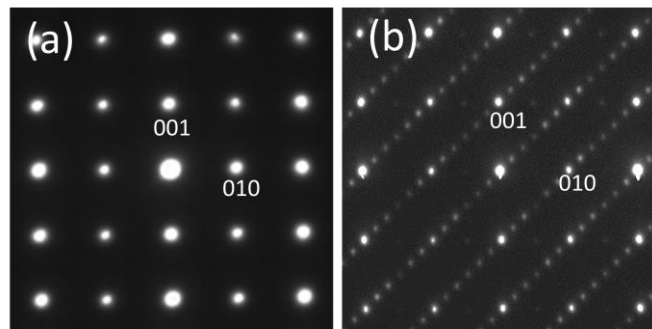


Figure 1: SAED patterns of (a) $\text{Al}_{72.5}\text{Rh}_{27.5}$  and (b) $\text{Al}_{74.5}\text{Rh}_{25.5}$  along  $[100]$ .

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## Interfacial stability for Quasicrystals-dispersed Mg alloys in Mg-Cd-Yb system

Satoshi Ohhashi<sup>1</sup>, Nobuhisa Fujita<sup>1</sup>, Akira Kato<sup>2</sup>, and An Pang Tsai<sup>1</sup>

<sup>1</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577, Japan*

<sup>2</sup>*Advanced materials engineering div., Toyota Motor Corporation, Susono 410-1193, Japan*

Mg alloys, well known as light materials, have been applied widely for PC, camera, chassis of car etc. Quasicrystals (Qc)-dispersed Mg alloys have been prepared in the Mg-Zn-Y system [1, 2], the Mg-Zn-Zr system [3], especially, excellent mechanical properties have been shown in Mg-Cd-Yb system [4]. It is supposed to be due to stable interface between Qc and  $\alpha$ -Mg phase [5]. In this work, evaluating the relationship of the stability and lattice matching, i.e. matching of peaks in XRD for the interface between Qc and Mg, we have estimated the energy profile for Fibonacci chain, intervals: 1 and  $\tau$  ( $\tau$ =golden ratio), average interval ( $a$ ):  $a=3/\tau-1$ , embedded in a periodic sinusoidal potential with periodic  $c = a/x$  ( $x$ =relative position of the Fibonacci chain along to the periodic potential). Large stabilization have been occurred in the case of  $a/x = 1$ , it could support the relationship of stability and the lattice matching for Qc /  $\alpha$ -Mg interface in the Mg-Cd-Yb system. In addition, Qc particles-dispersed Mg alloys could be fabricated successfully by solution treatment and re-precipitation methods. Qc particles with the size of 50~100 nm in the Mg matrix possess clear facets and orientation relationship to the matrix. This might be attributed to the stable interface between Qc and  $\alpha$ -Mg phase, expected to design the microstructure and mechanical properties.

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## Templated Quasicrystalline Molecular Layers

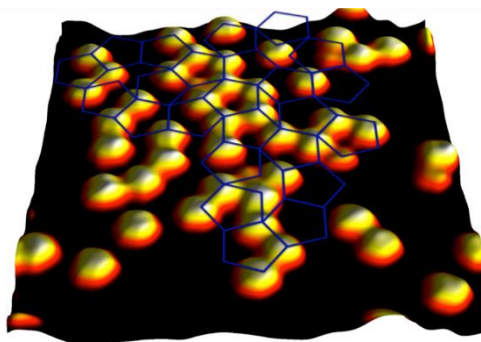
J. A. Smerdon<sup>1</sup>, K. M. Young<sup>2</sup>, M. Lowe<sup>2</sup>, S. S. Hars<sup>2</sup>, T. P. Yadav<sup>2</sup>, D. Hesp<sup>2</sup>, V. R. Dhanak<sup>2</sup>,  
A. P. Tsai<sup>3</sup>, H. R. Sharma<sup>2</sup> and R. McGrath<sup>2</sup>

<sup>1</sup>*Jeremiah Horrocks Institute for Mathematics, Physics and Astronomy, University of Central Lancashire, Preston, PR1 2HE, UK*

<sup>2</sup>*Department of Physics, University of Liverpool, Liverpool, L69 3BX, UK*

<sup>3</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577Japan*

Quasicrystals are materials with long range ordering but no periodicity [1]. We report scanning tunneling microscopy (STM) observations of quasicrystalline molecular layers on five-fold surfaces of icosahedral quasicrystals. The molecules adopt positions and orientations on the surface consistent with the quasicrystalline ordering of the substrate. Carbon-60 adsorbs atop sufficiently-separated Fe atoms on icosahedral Al-Cu-Fe to form a unique quasicrystalline lattice whereas further C<sub>60</sub> molecules decorate remaining surface Fe atoms in a quasi-degenerate fashion. Pentacene (Pn) adsorbs at tenfold-symmetric points around surface-bisected rhombic triacontahedral clusters in icosahedral Ag-In-Yb. These systems constitute the first demonstrations of quasicrystalline molecular ordering on a template.



*Figure 1: 3D representation of STM data collected from Carbon-60 adsorbed on five-fold Al-Cu-Fe.*

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## Icosahedral quasicrystal and approximant phases in Au-(Ga, Si, Sn)-Yb alloy systems

Yoko Nakamura<sup>1</sup>, Takuya Kurihara<sup>1</sup>, Tsunetomo Yamada<sup>2</sup>, An Pang Tsai<sup>2</sup>

<sup>1</sup>*Department of Materials Processing, Graduate school of engineering, Tohoku University, Sendai, Miyagi, 980-8577, Japan*

<sup>2</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577Japan*

Several icosahedral quasicrystal (iQC) phases containing Yb have been derived from the binary i-Yb-Cd [1]. Recently reported quantum criticality phenomenon in the i-Au-Al-Yb phase [2, 3] attracts a lot of interest in searching for new Yb-based iQC phases containing Au. In this presentation we report formation of a new iQC phase in Au-Sn-Yb alloy system. The single-grained iQC was synthesized by self-flux technique that exhibited dendritic form with pentagonal dodecahedron morphology. Reciprocal layers reconstructed from the single-crystal X-ray diffraction demonstrate that the obtained phase has icosahedral symmetry. The detailed formation condition of the iQC phase, as well as 2/1 and 1/1 periodic approximant phases found in Au-(Ga, Si, Sn)-Yb alloy systems will be presented.

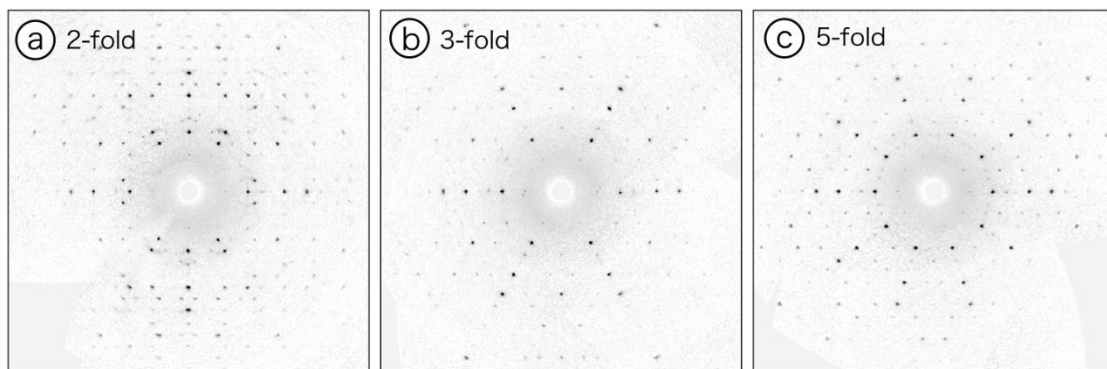


Figure 1; Reconstructed reciprocal layers from single-crystal x-ray diffraction for a single grained crystal in Au-Sn-Yb alloy.

Acknowledgement: The authors are grateful to Dr Y. matsushita and Mr A. Sato at NIMS for their helps during the diffraction experiment.

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## **Hard X-ray photoelectron spectroscopy (HAXPES) studies on quasicrystals and approximant crystals**

Masahiko Shimoda<sup>1</sup> and An Pang Tsai<sup>2</sup>

<sup>1</sup>*Research Center for Advanced Measurement and Characterization, National Institute for Materials Science (NIMS)*

*1-2-1 Sengen, Tsukuba, Ibaraki, 305-0047, Japan*

<sup>2</sup>*Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577Japan*

Hard X-ray Photoelectron Spectroscopy (HAXPES) is recognized as a powerful tool for studying properties of various materials. High energy photons provided by synchrotron radiation make it possible to probe electronic structures deep inside the bulk where the influence from the surface is negligible. In addition, this technique can detect deep core-levels of high binding energies with very high energy resolution. These features are unable to be realized by the conventional laboratory XPS measurements. Thus, it is well worth revisiting photoemission studies on quasicrystals with using this new technique, because most of previous works on photoemission were performed with using laboratory XPS. In this work, we will present recent HAXPES studies on quasicrystals, mainly on Al-based icosahedral quasicrystals such as i-Al-Pd-Mn.

## Evaluation of structural defects using positron annihilation study for 1/1-AIReSi approximant crystals made by spark plasma sintering

K. Yamada<sup>1</sup>, R. Maeda<sup>1</sup>, H. Suzuki<sup>1</sup>, H. Kitahata<sup>1</sup>, Y. Matsushita<sup>1</sup>, K. Nozawa<sup>2</sup>, F. Komori<sup>2</sup>, Y. Takagiwa<sup>3</sup>, K. Kimura<sup>4</sup>, and I. Kanazawa<sup>1</sup>,

<sup>1</sup>*Department of Physics, Tokyo Gakuai University, Tokyo 184-8501, Japan*

<sup>2</sup>*The Institute for Solid State Physics, the University of Tokyo, Chiba 277-8581, Japan*

<sup>3</sup>*National Institute for Materials Science (NIMS), Ibaraki 305-0047, Japan*

<sup>4</sup>*Department of Advanced Materials Science, the University of Tokyo, Chiba 277-8561, Japan*

1/1-AIReSi approximant crystals have attracted attention that temperature dependence of electrical resistance varies from metallic to semiconducting properties when increasing the concentration of Re [1]. It was shown that the Re occupancy at transition metal sites affected the electrical resistivity. Moreover, the crystal structure analysis in the case of changing the concentration of Al and Si was performed and this meant that the number of vacancies of glue sites varied [2]. However, the different crystal structure of Re concentration remains unresolved. In this study, we investigated the relationship between vacancies and electrical properties for 1/1-AIReSi. Since the microstructures of 1/1-AIReSi become porous due to anneal, we improved them by spark plasma sintering (SPS).

1/1-AIReSi ingots ( $\text{Al}_{73}\text{Re}_{17}\text{Si}_{10}$  and  $\text{Al}_{73}\text{Re}_{15}\text{Si}_{12}$ ) were prepared under an argon atmosphere with an arc-melting furnace and annealed in quartz tubes for 24 hours at 1023 K and for 48 hours at 1073 K, respectively. After that, the quartz tubes enclosing these ingots were quenched in water. To improve the microstructure of these ingots, each broken sample powder was sintered by SPS and then sintered samples were annealed for 24 hours at 1023 K. The qualities of the approximant crystalline phase were confirmed by X-ray diffraction analysis at room temperature. The resistivity was measured by the four probe method in the range between 10 K and room temperature. The structural defects were evaluated by the slow variable mono-energetic positron beam for Doppler broadening measurements.

The sintered samples of  $\text{Al}_{73}\text{Re}_{17}\text{Si}_{10}$  and  $\text{Al}_{73}\text{Re}_{15}\text{Si}_{12}$  were shown almost single phase and their temperature dependence of electrical resistance corresponds to semiconducting and metallic properties, respectively. From the results for sintered samples by positron annihilation studies, the values of S-parameter of the surfaces and inside of both samples did not vary. This implied that oxide affects inside of samples.

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## Adsorption structure of Bi on the fivefold surface of i-Ag-In-Yb quasicrystal

Kazuki Nozawa<sup>1</sup> and Yasushi Ishii<sup>2</sup>

<sup>1</sup>*Department of Physics and Astronomy, Kagoshima University, Kagoshima 890-0065, Japan*

<sup>2</sup>*Department of Physics, Chuo University, Tokyo 112-8551, Japan*

Recently, we reported three-dimensional growth of quasicrystalline Pb on the fivefold surface of the i-Ag-In-Yb quasicrystal used as a template [1]. The first-principles calculation based on the density functional theory revealed that adsorbed Pb atoms reconstruct the rhombic triacontahedral (RTH) cluster, the building block of the substrate quasicrystal, truncated by the surface [1]. It means that the atomic arrangement of the Pb layers is essentially same as the substrate. However, it is unclear why the multi-layered single-element quasiperiodic layers are obtained in this system, and also there is no guarantee that Pb is the best adsorbate for epitaxial growth on this substrate.

In this study, in order to find out differences depending on the adsorbate, we investigate the adsorption structure of Bi on the fivefold surface of i-Ag-In-Yb using the first-principles calculation, where Bi is one of the few elements proved to be forming a quasiperiodic monolayer on quasicrystalline substrates [2]. At the initial stage of deposition of Pb, we found five clear stable adsorption sites forming a pentagon of about 9 Å edge length around the center of the RTH cluster truncated by the surface [1, 3]. These stable sites forming the pentagon are originated from the 4th-shell of the RTH cluster surrounding the above-mentioned RTH cluster. For Bi, besides the pentagonal stable sites, another two pentagonal stable sites are found, which are also originated from the atomic sites of the substrate. Unlike the Pb case, the additional stable sites in the potential energy surface of Bi have comparable adsorption energy with the most stable pentagonal sites, meaning the different adsorption structure is expected for Bi and Pb. Details of the expected adsorption structure of Bi will be presented.

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## Crystalline approximants in the Al-rich part of the Al-Ru-Ni system

Shota Suzuki<sup>1</sup>, Rayko Simura<sup>1</sup>, Kazumasa Sugiyama<sup>1</sup> and Akira Yoshiasa<sup>2</sup>

<sup>1</sup>*Institute for Materials Research (IMR), Tohoku University, Sendai, Aoba-ku 980-8577 Japan*

<sup>2</sup>*Graduate School of Science and Technology, Kumamoto University, Kumamoto, 860-8555, Japan*

Since a stable decagonal phase was observed in the Al-Ru-Ni system [1,2], the Al-rich part of this ternary system was extensively studied by German group [3,4]. According to their reports, five stable ternary crystalline phases were identified in the Al-rich part of the Al-Ru-Ni phase diagram. They are *m*-AlRuNi (isostructural to Al<sub>9</sub>Co<sub>2</sub>), *M*-AlRuNi [5] (isostructural to Al<sub>13</sub>Ru<sub>4</sub>), *O*-AlRuNi [6] (isostructural to *O*-Al<sub>13</sub>Co<sub>4</sub>), hexagonal with a composition Al<sub>76</sub>Ni<sub>16</sub>Ru<sub>8</sub> ( $a=1.213\text{nm}$  and  $c=2.702\text{nm}$ ), and cubic with a composition Al<sub>72</sub>Ru<sub>17</sub>Ni<sub>11</sub> ( $a=0.767\text{ nm}$ , isostructural to *C*-Al<sub>5</sub>Rh<sub>2</sub>). Since the structural information on the crystals realized nearby quasicrystals, allows us to provide a useful idea for the atomic arrangement, single crystal X-ray diffraction study for the five stable crystals is very important. The present paper reports the results of structural analysis for two remaining Al-Ni-Ru phases.

Alloy ingots with the chemical compositions of Al<sub>71</sub>Ru<sub>16</sub>Ni<sub>13</sub> and Al<sub>76</sub>Ni<sub>16</sub>Ru<sub>8</sub> were prepared by using a conventional arc-melting furnace under purified argon atmosphere. The structure of *C*-AlRuNi is similar to that of *C*-Al<sub>5</sub>Rh<sub>2</sub> by showing a pseudo-Mackay cluster (pMC) and a mini Bergman cluster (mBC). In particular, the pMC consists of three shells; an Al-icosahedron with a Ru/Ni-center, a Ru/Ni- icosahedron and an Al-icosidodecahedron. The structure of (*H* or *T*)-AlNiRu is similar to that of  $\chi$ -AlReRu (*P31c*,  $a=1.237\text{nm}$ ,  $c=2.749\text{nm}$ ) [7] and the pMC with a disordered first shell was found in the structure.

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## Reinvestigation of 'Dy<sub>5</sub>Pd<sub>2</sub>', crystal structure of Dy<sub>71.17</sub>Pd<sub>24.48</sub> (~Dy<sub>5.81</sub>Pd<sub>2</sub>)

Yoshitaka Matsushita<sup>1</sup>, Saori Toyozumi<sup>1,2</sup>, Hideaki Kitazawa<sup>1</sup>,  
Kengo Morita<sup>2</sup>, Akira Tamaki<sup>2</sup>, and Satoshi Kawada<sup>1</sup>

<sup>1</sup>National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047,  
Japan

<sup>2</sup>Tokyo Denki University, 5 Senju Asahi-cho Adachi, Tokyo 120-8551, Japan

Recently, magnetic refrigeration using magnetocalorimetric effect (MCE) is pointed as an energy-efficient refrigeration technology. Especially, the MCE phenomena may be useful for hydrogen liquefaction. These days, compounds so-called ' $Ln_5Pd_2$ ' ( $Ln = Y$  and heavier lanthanoid elements such as Tb, Dy, Ho, Er, Tm, Lu) are focusing on as potential materials for magnetic refrigeration with MCE. For an example, 'Ho<sub>5</sub>Pd<sub>2</sub>', shows spin-glass behaviour below 26.7 K [1], and around the temperature the compound shows large MCE [2]. To understand origin and relation of such properties, detail information of its crystallographic and magnetic structures is necessary. In the previous structure report, the so-called ' $Ln_5Pd_2$ ' ( $Ln = Y$  and heavier lanthanoid elements such as Tb, Dy, Ho, Er, Tm, Lu) compounds have an original crystal structure type: cubic Dy<sub>5</sub>Pd<sub>2</sub>-type structure. The type of crystal structure shows heavily site disordered behaviour. [2, 3] Thus the structural composition of Dy<sub>5</sub>Pd<sub>2</sub> is Dy<sub>68</sub>Pd<sub>28</sub> (~Dy<sub>4.86</sub>Pd<sub>2</sub>). This site disorder seems to be related to the properties. However, detail of crystal structure of this compound is still unclear. Therefore, its crystal structure was reinvestigated by single crystal X-ray diffraction method.

Single crystals of the title compound were grown by non-seed crystal pulling method in a tetra-arc furnace under Ar atmosphere. Structure study was carried out Rigaku AFC11 Saturn724+ CCD diffractometer at 293 K. Resulted space group and cell parameter are Fd-3m and  $a = 13.5087(11)$  Å, respectively. As preliminary structure model, we used the previously reported model. [3] However, many of maximum and minimum electron densities were still existed around Pd site and Ho1 site with high  $R$  value ( $> 8\%$ ). Therefore, heavier disordering model was applied, and renamed all crystallographic sites. Then, the final  $R$  value drastically was dropped to 3.54%. The details will be presented.

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## Surface structure and epitaxy on Ag-In-RE quasicrystals and related periodic approximants

H. R. Sharma<sup>1</sup>, S. Hars<sup>1</sup>, J. A. Smerdon<sup>1</sup>, S. Thorn<sup>1</sup>, A. Al-Mahboob<sup>1</sup>, Smerdon<sup>1</sup>, K. Nozawa<sup>2</sup>, Y. Ishii<sup>2</sup>, R. Tamura<sup>3</sup>, A. P. Tsai<sup>4</sup> and R. McGrath<sup>1</sup>

<sup>1</sup>The University of Liverpool, Department of Physics, Liverpool, UK; <sup>2</sup>Chuo University Tokyo, Japan; <sup>3</sup>Tokyo University of Science, Japan; <sup>4</sup>Tohoku University, Japan

We present our recent studies on surfaces and epitaxy on the Cd-Yb type quasicrystals and related periodic approximants. The systems used in this study are Ag-In-RE (RE: Yb, Tb and Gd) approximants and icosahedral (*i*) Ag-In-Yb quasicrystal, which are isostructural to the Cd-Yb phases with Cd replaced by Ag and In. The surfaces of these systems can be prepared with large atomically flat terraces which correspond to the truncation of rhombic triacontahedral (RTH) clusters, the building block of these systems. The approximants develop facets along different crystallographic directions. Interestingly though, there are some common features in all surfaces. It is suggested that bonding between electronic states of In and RE may play role for stability of the surfaces [1].

We will also present our recent observations of templated quasicrystalline order of single elements (Pb, Bi and In) and molecules (pentacene and C<sub>60</sub>) (Figure 1). Using scanning tunnelling microscopy (STM) and DFT calculations, we find that the adsorbates occupy the positions of the RTH cluster [2]. We also observe that pentacene molecules adsorb at tenfold-symmetric sites of Yb atoms around surface-bisected RTH clusters, yielding quasicrystalline order [3]. Similarly, C<sub>60</sub> growth on *i*-Al-Cu-Fe also produces quasicrystalline layer, where the growth is mediated by Fe atoms on the surface [3].

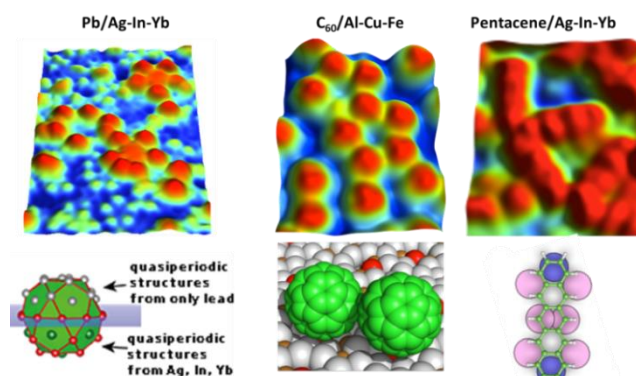


Figure 1: STM observation of quasicrystalline thin film of Pb, C<sub>60</sub> and Pentacene formed on the quasicrystal surfaces.

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## Metal ions, solvent effects, hydrogen bonding, electronic structure and topology in G-quadruplex DNA

Lokendra Poudel<sup>1</sup>, Nicole F. Steinmetz<sup>2,3</sup>, Roger H. French<sup>3</sup>, V. Adrian Parsegian<sup>4</sup>, Rudolf Podgornik<sup>4</sup>, Wai-Yim Ching<sup>1</sup>

<sup>1</sup>*Department of Physics and Astronomy, University of Missouri-Kansas City, Kansas City, MO 64110, USA*

<sup>2</sup>*Department of Biomedical Engineering, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106, USA*

<sup>3</sup>*Department of Materials Science and Engineering, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, OH 44106, USA*

<sup>4</sup>*Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003, USA*

The G-quadruplex DNAs (G4-DNA) are planar four-stranded DNA structures derived from repetitive guanine-rich nucleic acid sequences connected by Hoogsteen hydrogen bonding (HB) between a tetrad of guanine bases [1]. There is intense interest in the properties of G4-DNAs because of their importance in biomedical science, potential applications in biotechnology and the role it can play in energy-relevant materials [2]. We present a *first-principles* density functional study elucidating the effects of solvent, metal ions and topology on the electronic structure and hydrogen bonding of 12 well-designed G-quadruplex (G4-DNA) models in different environments. Our study shows that the parallel strand structures are more stable in dry environment and aqueous solutions containing  $K^+$  ions within the tetrad of the guanine but conversely, that the anti-parallel structure is more stable in solutions containing the  $Na^+$  ions within the tetrad of the guanine. The presence of metal ions within the tetrad of the guanine channel always enhances the stability of the G4-DNA models. The parallel strand structures have larger HOMO-LUMO gaps than antiparallel structures, which are in the range of 0.98 eV to 3.11 eV. The comparative study between specific pairs of different G4-DNA models shows that the Hoogsteen O $\cdots$ H and N $\cdots$ H hydrogen bonds in the guanine tetrad are significantly influenced by the presence of metal ions and water molecules, and collectively affecting the structure and stability of G4-DNA.

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## Magnetism in zigzag and armchair CuO nanotubes: Ab-initio study

Samir Paudel<sup>1</sup>, Gopi Chandra Kaphle<sup>2</sup>, and Anurag Srivastava<sup>3</sup>

<sup>1</sup>*Department of Physics, Tribhuvan University, Patan Multiple Campus, Patan Dhoka, Lalitpur, Nepal*

<sup>2</sup>*Central Department of Physics, Tribhuvan University, Kathmandu, Nepal.*

<sup>3</sup>*ABV-Indian Institute of Information Technology and Management, Gwalior, M.P., India.*

Metal oxide semiconductors are among the most promising material for future electronic, optical and magnetic applications. Among the other metal oxides, CuO demonstrated itself as a future candidate for spintronics, data storage and magnetic sensor devices. In the present study, the diameter dependence structural stability, electronic and magnetic properties of zigzag (n, 0) ( $4 \leq n \leq 12$ ) and armchair (n, n) ( $3 \leq n \leq 8$ ) copper oxide nanotubes (CuO NTs) have been analyzed by employing a standard density functional theory based ab-initio approach using spin polarized generalized gradient approximation with revised Perdew Burke Ernzerhoff type parameterization. By increasing the diameter of nanotube with help of Chirality, Different parameters such as Structural analysis, binding energy, total magnetic moment and spin polarization have been calculated. The structural stability is examined by binding energy, optimized structure and optimized bond length between Cu and O atoms, where we observed that binding energy increases with increasing diameter for both zigzag and armchair CuO nanotubes. In the both geometry, zigzag and armchair nanotubes, copper and oxygen atom form a homocentric cylinder with different diameter  $D_{Cu-Cu}$  and  $D_{O-O}$ , denotes the diameter of copper and oxygen cylinder respectively. The observed buckling on the structure of NTs is perceived to be decreasing with increasing diameter of the Nanotube. Both Optimized buckled geometry of zigzag and armchair nanotubes shows that the  $D_{O-O}$  is greater than  $D_{Cu-Cu}$ . The calculated total magnetic moment is observed to be decreased with increasing diameter of CuO nanotubes. Among the considered chiralities, (5, 5) armchair (diameter 9.08 Å) and (9, 0) zigzag (diameter 9.47 Å) CuO nanotubes are found to have highest degree of spin polarization, however total magnetic moment is found to be high for (4, 0) zigzag and (3, 3) armchair CuO NTs. The computed electronic properties of considered CuO NTs conform the metallic nature of these nanotubes.



## First-principles study of a molecular adsorption of water on MoS<sub>2</sub>/graphene bilayer hetero-structure

Hari Paudya<sup>1</sup>, [Narayan Prasad Adhikari](#)<sup>1</sup> and Biplab Sanya<sup>2</sup>

<sup>1</sup>*Central Department of Physics, Tribhuvan University, Kathmandu, Nepal.*

<sup>2</sup>*Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box-516, SE 75120 Sweden.*

We have performed the first-principles calculations to study the stability, geometrical structure and electronic properties of pure MoS<sub>2</sub> monolayer, MoS<sub>2</sub>/Graphene bilayer hetero-structures (MGBHs) and a water molecule adsorbed MGBHs based on the Density Functional Theory (DFT) with van der Waals (vdW) interactions in the DFT-D2 approach under Generalized Gradient Approximation (GGA). Our findings show that the MoS<sub>2</sub> monolayer is stable direct band gap semiconductor with binding energy (B.E)/MoS<sub>2</sub> molecule 11.36 eV and band gap of 1.14 eV. The planer distance MGBHs is also found stable with the B.E of 1.083 eV at 3.37 Å between MoS<sub>2</sub> and graphene layers. Moreover, we have studied the B.E of a water molecule at different sites of MGBHs and found that the hollow position of hexagonal ring of the graphene sheet is the most favorable site for the adsorption from the graphene plane and at with the B.E of 0.123 eV at a distance of 2.86 Å 3.25 Å from the nearest C-atom. The band structure analysis of MGBHs shows that the system is metallic and the band structure is nearly the sum of each constituents (i.e. MoS<sub>2</sub> +graphene). The states at the Fermi level are contributed solely by graphene, which demonstrates that the addition of graphene can significantly increase the conductivity of constituent monolayers. Due to the adsorption of a water molecule on MGBHs, it revealed new insights to a better understanding of the water molecular adsorption on the surface of 2D-materials. Further, the study of DOS calculation suggests pure MoS<sub>2</sub> monolayer, MGBHs and a water molecule adsorbed MGBHs as non-magnetic. The calculations of charge transfer shows a small charge shifting of magnitude 0.059e from graphene to MoS<sub>2</sub> in MGBHs and 0.0024e to H<sub>2</sub>O from the MGBHs in a water molecule adsorbed MGBHs. Finally, the effect on the electronic and magnetic properties on intrinsic atomic defect created MGBHs is studied with the adsorption of a water molecule.

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► Supported by: Swedish Research Links.

## **Electronic structures and concentration dependent magnetism on NiGa and Ni<sub>3</sub> Ga**

S. Lamichhane, G. C. Kaphle, and N.P. Adhikari

*Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal*

The Ni rich NiGa alloys which exhibit the magnetism are widely used in the high technology applications. We have studied the electronic structures and magnetism related aspects of ordered NiGa and Ni<sub>3</sub>Ga using the tight-binding linear muffin-tin orbitals atomic sphere approximation included in TB LMTO-ASA approach. We went through the band structure calculations to visualize the wave-vector dependence of energy states along with possible electronic transition and to know the contributions of the orbitals in the bands. Our findings show that all the system considered are metallic in nature. Furthermore, spin up and spin down calculations have been done to know the magnetic properties of the system. The nickel is, of course magnetic while NiGa is found to be nonmagnetic, Ni<sub>3</sub>Ga is, however, weak ferromagnet. Appearance of Ni in Ni<sub>3</sub>Ga alloy contributes to display effective magnetic moment of 0.58  $\mu_B$  showing the dominant factor towards magnetism. The partial density of states were also investigated to analyze the strength of p-d hybridization. The value of magnetic moment of Ni<sub>3</sub>Ga obtained in the present work agrees with previous studies.

Keywords : Atomic Sphere Approximation; Hybridization; Magnetism; Binary alloys

## **First-principles study of electronic and magnetic properties of manganese decorated graphene**

Bishnu Prasad Paudel, Nurapati Pantha, and Narayan Prasad Adhikari

*Central Department of Physics, Tribhuvan University Kirtipur, Kathmandu, Nepal*

The functionalization of graphene by the addition of Manganese (Mn) atom to its surface has been investigated by using density-functional theory (DFT) based first-principles method within DFT-D2 level of approximations. The calculations have been computed employing the Quantum ESPRESSO codes. The stability, geometrical structures, electronic and magnetic properties of pure and Mn adatom graphene systems have been studied. From the information of adsorption energies of Mn atom on the different sites of graphene, the top site is found to be the most favorable one for its adsorption. Present study finds that the London dispersion interaction plays a major role in the weak binding of Mn on graphene. The study of electronic and magnetic properties of Mn decorated graphene shows that the conduction and valence band are overlapped with finite density of states (DOS) at Fermi level. The dissimilar DOS for up and down spin calculations quantify magnetic moment as 5.48  $\mu\text{B}$  which is consistent with the previous study. Keywords: DFT; Magnese; quantum espresso; band structure

## **The comparison of magnetic and physical properties of quasicrystals with their constituting elements**

Maryam Kiani and Feridoun Samavat

*Department of Physics, Faculty of Science, BuAli Sina University, Hamadan, Iran*

In this paper, the properties of quasicrystals will be discussed. At first, it considers the physical and mechanical properties of quasicrystals, and compares them with the properties of Aluminum, mainly since their composition often contains 60%-70% Aluminum; thus, their properties can be dependent upon the element Aluminum. Then, electrical and magnetic properties of the noted substances are compared with the characteristic properties of Iron.

Their magnetic and electrical properties have been investigated and compared because the amorphous structure is often correlated with the icosahedral structure. The magnetization, which is measured up to 300kOe [1] for the amorphous alloys, are slightly larger than those of the quasicrystalline alloys, and the paramagnetic Curie temperature of the former alloys is larger than that of the latter alloys [1]. The magnitude of effective magnetic moment  $P_{\text{eff}}$  determined from the Curie-Weiss law for crystalline alloys is qualitatively explained in terms of the Pauling valence. The value of  $P_{\text{eff}}$  of the quasicrystalline alloys is the same as that of the amorphous ones and about two times that of the crystalline alloys with the same composition [1].

Therefore, the magnitude and the temperature dependence of electrical resistivity of the quasicrystalline alloys are very different from those of the crystalline alloys. The results of measurements show that by annealing the electric resistance in quasicrystals dramatically decreases. And this would be due to the fact that, as Al-Pd-Mn sputtered for long period of time, the concentration of Mn is decreased during annealing and this confirms our result for magnetic properties. [2, 3]. week magnetic properties in quasicrystals is because of the existence of Mn element, as the LEIS measurements [3], calculation and measurement of LEED show the low concentration of Mn in surface and layer. Electric resistance depends on the concentration of Mn and its variation due to the temperature is like amorphous materials.

[1] K. Fukamichi and T. Goto. , Science reports of the Research Institutes, Tohoku University. Ser. A, Physics, chemistry and metallurgy, 34.2, 267 (1989).

[2] C. J. Jenks, J.W. Burnett, D. W. Delaney, T. A. Lograsso, & P. A. Thiel, Applied surface science 157.1, 23 (2000).

[3] F. Samavat et al, Surface and Interface Analysis 40.3-4,433 (2008).

## **Study of deposition method of the each Al, Pd elements on the Al-Pd-Mn quasicrystal**

Maryam Kiani and Feridoun Samavat

*Department of Physics, Faculty of Science, BuAli Sina University, Hamadan, Iran*

In this work, Pd element has been deposited on the clean surface Al-Pd-Mn quasicrystal by evaporated and using low energy ion scattering (LEIS) technique [1] and similar experiments were done for Al. LEIS technique is usually used for surface analysis because it is very sensitive to the topmost layer on the sample and this property makes it as a unique technique for surface analyzing.

At first the sample prepared through a combination of sputtering and annealing. Then the Pd monolayer was deposited on the surface and measured the ratio of Al/Pd for clean annealed surface at the room temperature. Drawing the Al/Pd ratio versus time deposition the obtain graph is the linear. That shows Pd growth is Layer Growth (Frank-Van der-Merwe Growth). Similar experiment for Al has done, and also study by Sharma et al. [2] and results show that growth the Al on the sample is also is Layer Growth (LG).

[1] F. Samavat, B.V. King, and J. O'Connor. *Surface Review and Letters*, 14.01, 31 (2007).

[2] H. R. Sharma, M. Shimoda, and A. P. Tsai. *Advances in Physics*, 56.3, 403 (2007).

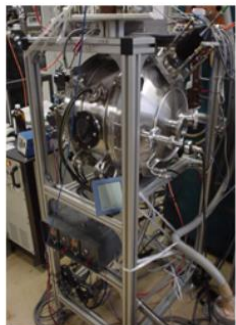
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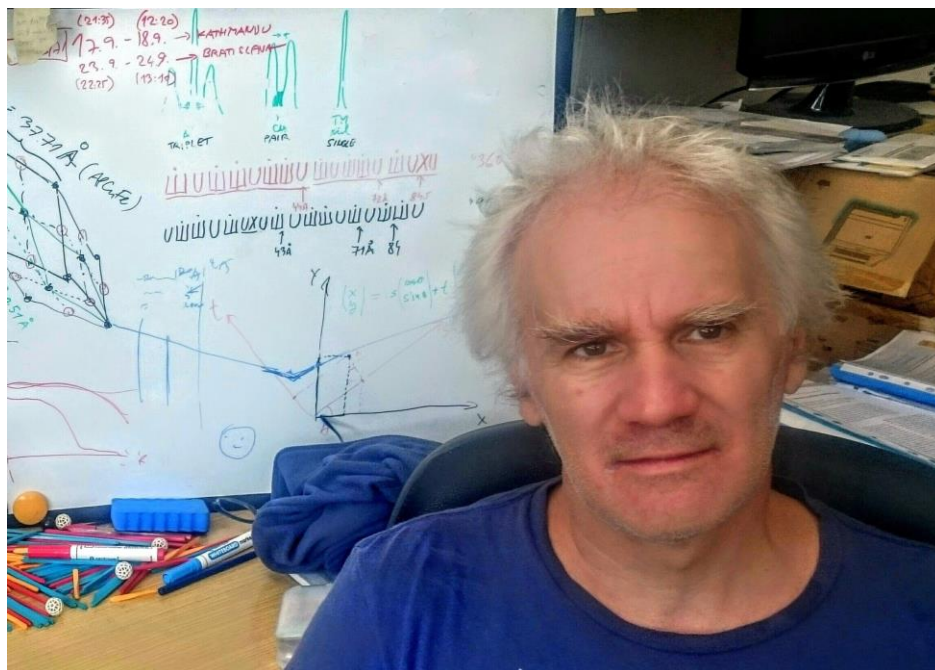


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## Dubois Award 2016

The International Advisory Board of the Thirteenth International Conference on Quasicrystals has announced to award DR MAREK MIHALKOVIČ the Jean Marie Dubois Award 2016 for Excellence in Quasicrystal Research.



Dr. Marek Mihalkovič earned his M. Sc. degree (equivalent) in 1987 at the Faculty of Mathematics and Physics of Comenius University in Bratislava. He earned his Ph.D. (equivalent) in 1989 at the Institute of Physics at the Slovak Academy of Sciences, with a dissertation on the “Structure of Icosahedral Quasicrystals.” He is now an independent researcher at the Institute of Physics in the Department of Physics of Metals, a part of the Slovak Academy of Sciences. Dr. Mihalkovič has been a visiting scientist or visiting professor at several institutions, including the Technische Universität Chemnitz, Cornell University, Carnegie Mellon University, SIMAP Grenoble, and AGH Krakow. His research on, or related closely to, quasicrystals has ranged from atomic dynamics, optimization of complex atomic structures, and studies of phase stability. In 2016 at ICQ13, he will receive the Jean Marie Dubois Award “for theoretical work that has enabled and demonstrated the simulation of thermodynamic and dynamic properties of quasicrystals, based on realistic atomic-scale models and energetics.”



## List of Participants

<b>Name</b>	<b>Institute</b>	<b>Country</b>
Agnieszka Wolny	AGH University of Science and Technology	Poland
Akihisa Koga	Tokyo Institute of Technology	Japan
Akira Yoshiasa	Kumamoto University	Japan
Alan I Goldman	Iowa State University/ Ames Laboratory	USA
Alok Singh	National Institute for Materials Science	Japan
An Pang Tsai	Tohoku University	Japan
Andreas Kreyssi	Ames Laboratory, Iowa State University	USA
Antoine Julien	Nord University	Norway
Anuradha Jagannathan	Universite Paris-Sud	France
Asuka Ishikawa	Tokyo University of Science	Japan
Aya Yubuta	Tohoku University	Japan
Bishnu Prasad Paudel	Tribhuvan University	Nepal
Carmela Yaroslavski	Ben-Gurion University of the Negev	Israel
Cesar P Gomez	Angstrom Laboratory, Uppsala University	Sweden
Chuang Dong	Dalian University of Technology	China
Chul-Sik Kee	Advanced Photonics Research Institute, GIST	Republic of Korea
Dan Liu	SIMaP, University Grenoble Alpes	China
Dan Shechtman	Technion, Israel Institute of Technology	Israel
Daniela Wolny	AGH University of Science and Technology	Poland
Dmitry Shulyatev	National University of Science and Technology MISIS	Russia
Dvir Flom	Ben-Gurion University of the Negev	Israel
Eiji Abe	University of Tokyo	Japan
Elena Y. Vedmedenko	University of Hamburg	Germany
Emilie Gaudry	Institut Jean Lamour, Universite de Lorraine CNRS	France
Esther BELIN-FERRE	CNRS Institut Jean Lamour	France
Fang Fang	Quantum Gravity Research	USA
Feriduon Samavat	Bu-Ali Sina University	Iran
Guillaume Cini	Institut Jean Lamour, CNRS-Universite de Lorraine	France
Guy Trambly de Laissardiere	LPTM, Univ. Cergy-Pontoise, CNRS	France
Hadi Parsamehr	National Tsing Hua University	Taiwan
Hans-Rainer Trebin	University of Stuttgart	Germany
Hari Prasad Dahal	American Physical Society	USA
Hem Raj Sharma	University of Liverpool	United Kingdom

Hiroyuki Takakura	Hokkaido University	Japan
Ingeborg Waltraud Weller	University of Stuttgart	Germany
Ireneusz Jozef Buganski	AGH University of Science and Technology	Poland
Ivona Cernickova	Slovak University of Technology	Slovakia
Janez Dolinsek	Jozef Stefan Institute	Slovenia
Janusz Wolny	AGH University of Science and Technology	Poland
Jean-Marie DUBOIS	CNRS Institut Jean Lamour	France
Jing Chen	Dalian University of Technology	China
Joanne M Goldman	Iowa State University/ Ames Laboratory	USA
Joe Smerdon	University of Central Lancashire	United Kingdom
Joseph William Firth	University of Leeds	United Kingdom
Julian Ledieu	Institut Jean Lamour, Universite de Lorraine CNRS	France
Junji YUHARA	Nagoya University	Japan
Kaoru Kimura	The University of Tokyo	Japan
Katariina Pussi	Lappeenranta University of Technology	Finland
Kazue Nishimoto	IMRAM, Tohoku Univ.	Japan
Kazuhiko Deguchi	Nagoya University	Japan
Kazuki Nozawa	Kagoshima University	Japan
kazumasa Sugiyama	IMR, Tohoku University	Japan
Keiichi Edagawa	Institute of Insustrial Science, Univ. Tokyo	Japan
Klee Irwin	Quantum Gravity Research	USA
Kohei Yamada	The University of Tokyo,	Japan
Koichi Kitahara	The University of Tokyo	Japan
Kotoba Toyonaga	Hokkaido University	Japan
Latham Boyle	Perimeter Institute for Theoretical Physics	Canada
Lax Chan	The Open University	United Kingdom
Libor Duriska	Slovak University of Technology	Slovakia
Lokendra Poudel	University of Missouri-Kansas City	USA
Ma. Lailani B. Walo	University of the Philippines	Philippines
Maciej Stefan Chodyn	AGH University of Science and Technology	Poland
Marc de Boissieu	Simap CNRS Universite Grenoble Alpes	France
Marek Adamech	Slovak University of technology	Slovakia
Marek Mihalkovic	Slovak Academy of Sciences (IP SAS)	Slovakia
Maria Klyueva	National University of Science and Technology MISIS	Russia
MarkHankowski	Suneidon Corporation	USA
Maryam Kiani	Bu-Ali Sina University	Iran
Masahiko Shimoda	National Institute for Materials Science	Japan

Michael Widom	Carnegie Mellon University	USA
Ming-Sheng Leu	Industrial Technology Research Institute, MCL	Taiwan
Monika Wolny	AGH University of Science and Technology	Poland
Narayan Prasad Adhikari	Tribhuvan University	Nepal
Natsu Ito	Tokyo University of Science	Japan
Nayuta Takemori	CEMS, RIKEN	Japan
Nicolas Mace	Universite Paris-Sud	France
Nicolino Biagio Lo Gullo	Universita degli Studi di Milano	Italy
Nilay Krishna Mukhopadhyay	Indian Institute of Technology (BHU)	India
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Ryota Maeda	Tokyo Gakugei University	Japan
Ryuji Tamura	Tokyo University of Science	Japan
Sam Coates	University of Liverpool	United Kingdom
Samir Paudel	Tribhuvan University	Nepal
Saran Lamichhane	Tribhuvan University	Nepal
Shelomo Izhaq Ben- Abraham	Ben-Gurion University of the Negev	Israel
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Stefan Forster	Martin-Luther-Universitat	Germany
T.P. Yadav	Banaras Hindu University	India

Takanobu Hiroto	The University of Tokyo	Japan
Takanori Sugimoto	Tokyo University of Science	Japan
Takehiro Onodera	Tokyo Gakugei University	Japan
Tomonari Dotera	Kindai University	Japan
Tsunetomo Yamada	IMRAM, Tohoku University	Japan
Tsutomu Ishimasa	Hokkaido University	Japan
Uwe Grimm	The Open University	United Kingdom
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Walter Steurer	ETH Zurich	Switzerland
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Yoshitaka Matsushita	National Institute for Materials Science	Japan
Yujiro Tanaka	Tokyo University of Science	Japan
Yuuki Sekiyama	Tokyo Gakugei University	Japan
Zdenka Dolinsek	Jozef Stefan Institute	Slovenia
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