

APERIODIC'09

6th International Conference on
Aperiodic Crystals

Liverpool, 13 – 18 September 2009



Programme and Abstracts

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1 Welcome

Welcome to Liverpool and to Aperiodic'09.

Aperiodic'09 is the sixth International Conference on Aperiodic Crystals, organized under the auspices of the Commission on Aperiodic Crystals of the International Union of Crystallography (IUCr). It follows Aperiodic'94 (Les Diablerets), Aperiodic'97 (Alpe d'Huez), Aperiodic'2000 (Nijmegen), Aperiodic'03 (Belo Horizonte) and Aperiodic'06 (Zao).

Although UK scientists have made several important contributions to the field of Aperiodic Crystals, this is the first time that a major conference on the topic has been held in this country. About 110 participants are expected to attend, and we have assembled a full and varied scientific and social programme.

The following pages contain detailed information about the programme and the conference venues. We also included some general information on Liverpool and hope you will find some time to explore the city which was European Capital of Culture in 2008.

Members of the conference organising committee will be happy to assist you at any time during the meeting. Please feel free to approach them as necessary.

We wish you an enjoyable stay in Liverpool and a fruitful conference.

Ronan McGrath and Uwe Grimm (co-chairs)

2 Organisation

2.1 National Organising Committee

Rónán McGrath (University of Liverpool) (co-chair)
Uwe Grimm (Open University) (co-chair)
Steve Barrett (University of Liverpool)
Olga Degtyareva (University of Edinburgh)
Tim Noakes (Daresbury Laboratory)
Hem Raj Sharma (University of Liverpool)
Joe Smerdon (University of Liverpool)
Wolfgang Theis (University of Birmingham)
Angie Reid (conference secretary)

2.2 International Programme Committee

Nadezhda B Bolotina (Russia)
Gervais Chapuis (Switzerland)
Marc de Boissieu (France)
Dewei Deng (China)
Ron Lifshitz (Israel)
Gerardo G Naumis (Mexico)
J Manuel Perez-Mato (Spain)
Srinivasa Ranganathan (India)
Walter Steurer (Switzerland)
Patricia A Thiel (USA)
An Pang Tsai (Japan)
Ray Withers (Australia)
Sander van Smaalen (Germany)

2.3 International Advisory Board

The IUCr Commission on Aperiodic Crystals, chaired by Marc de Boissieu, acts as the International Advisory Board.

3 Sponsors

We are grateful to our sponsors:



The Open University



International Union of Crystallography



4 General information

- **Registration** Registration will be available at the Tutorial Session (see below), at the Welcome Party (see below) and during the conference at the Conference Office (9.30-15.00) in the Sherrington Suite. All registration queries concerning payments/receipts should be made at the conference office.
- **Tutorials** Tutorials will be held on Sunday at 14.00 in the Surface Science Research Centre.
- **Conference** The main conference location is the Sherrington Suite, lecture theatre 1. There will be a meeting office here for queries on the programme, social activities and proceedings. There is also a computer room available. Coffee breaks and lunches will be in the foyer area.
- **Oral presentations** Invited talks should be 30-35 minutes with an extra 5-10 minutes for questions. Contributed talks should be 15 minutes with an extra 5 minutes for questions. The lecture theatre computer is a Windows PC. Delegates are encouraged to use these but may also use their own machines. Please ensure your presentation is loaded before your session starts. Please keep to time as the timetable is very full. Your session chair will assist with time-keeping.
- **Poster sessions** Poster sessions will be held in the Science Project Laboratory in the Chadwick building. Light refreshments will be served at both sessions. Odd-numbered posters will be discussed on Tuesday evening, even-numbered on Thursday. Posters should be mounted before the session on Tuesday and taken down after the session on Thursday. Posters should be in Poster orientation, A0 size maximum.
- **Public Lecture** Prof. Sir Roger Penrose will deliver a lecture on Tuesday 15th Sept at 16.15. We will be joined by other members of the University for this lecture.
- **Internet access** Delegates may have guest access to the internet either via wireless, or by using a terminal in any of the University computer centres. There is a computer centre in the Sherrington suite. Dr. Hem Raj Sharma will assign an ID and password on request.
- **Proceedings** The proceedings will be published in the Journal of Physics Conference Series. A template is available on the conference website.
- **Student prizes** There will be two student prizes, one for the best student talk and one for the best poster presentation. Prizes will be presented at the closing session.
- **Banking, shops, cafes** A branch of Barclays Bank is located on Brownlow hill just past University square. There is a Tesco supermarket and a Costa Coffee on Brownlow hill just downhill from University square. The University bookstore, on University square, also has a cafe on the first floor.



MAP KEY

- Galleries & Museums**
 - 01 Merseyside Maritime Museum
 - 02 International Slavery Museum
 - 03 Maritime Museum
 - 17 The Beatles Story
 - 18 The Beatles Story
 - 26 Opening This Year
 - 47 Tate Liverpool
 - 48 Mermaid House
 - 49 Piermaster's House
- Bars & Restaurants**
 - 03 Outside Café
 - 04 The Pan American Club
 - 05 Gusto (formerly Est Est Est)
 - 06 Blue Bar & Grill / Baby Blue
 - 07 Babycream
 - 08 Hahai Bar & Canteen
 - 09 Spice Lounge
 - 14 Circo
 - 15 Coda Coffee
 - 21 Coda Wine Bar and Deli
 - 22 Raven
 - 23 The Pan American Club
 - 24 Opening This Year
 - 36 Nosh
 - 38 Hansel & Gretel's Take Away
 - 39 Hansel & Gretel's Cafe
 - 44 La Crepe Rit
 - 45 Tate Cafe
- Shops**
 - 13 FabStoner/Coffinhouse
 - 16 Interiors of Liverpool
 - 19 Narditalia
 - 27 Apple Centre/Canon
 - 29 Annabel's Accessories
 - 30 Quay Confectionery
 - 31 Art 4 You
 - 32 Liverpool Pictures
 - 33 Nature's Treasure
 - 35 Warehouse
 - 40 Whitelish Gallery
 - 41 The Gift Company
 - 46 Tate Shop
- Hotels**
 - 15 Premier Inn
 - 20 T Express
 - 25 Express by Holiday Inn
- Commercial**
- Residential**
- Services**
 - I Visitor Centre / Information
 - Smart Bus Stop
 - Disabled Parking
 - P Pay & Display Parking
 - Taxi Rank
 - Toilets & Baby Care
 - ATM cash machines. Also located in the basement of Tate Liverpool

5 Social events

- **Welcome reception** A welcome reception will be held in the Victoria Gallery and Museum off University Square on Sunday at 18.00. Registration will also be available.
- **Beer-tasting** English beer is weak, warm and soapy — or is it? Please join the beer-tasting event in the Augustus John pub just off University square on Monday at 18.00. You will be given two tickets which may be exchanged for drinks in the bar.
- **Excursion** The excursion will take place on Wednesday afternoon. Taxis will bring us to the ferry terminal for a 14.00 explorer trip round the Mersey. At 15.00 refreshments will be available in the bar at the ferry terminal. The ferry terminal also houses part of the Beatles exhibition. You will be given a ticket to enter (which you should retain for entry to the Beatles Story later), or you may choose to wander down to the Albert Dock area and visit the Maritime Museum, the International Museum of Slavery, or the Tate Gallery. All museums and Galleries on Merseyside are free to enter. Across the road from the Albert dock is Liverpool One, the newest and one of the most stylish shopping areas in the UK, opened in 2008. Both Liverpool FC and Everton FC have official souvenir shops here.

You will be assigned to one of four groups for a guided tour of the Beatles Story on the nearby Albert Dock. Entry will be at: 16.00, 16.20, 16.40 and 17.00. Afterwards there is some free time before the conference dinner.
- **Conference dinner** The Conference dinner will be held at the Crown Plaza hotel, near the Albert Dock. Drinks reception at 19.30, dinner at 20.00. Music will be supplied by renowned Liverpool singer Nick Lacey. He has also offered an “open microphone” should anyone feel inspired. Special guests are Prof. Alan Mackay and his wife Sheila. Dress is smart casual.

6 Hotels and directions

Liverpool has a busy but safe city centre. However, you should take appropriate care of yourself and belongings, as in any reasonably sized city.

Directions from hotels to venues:

- **Feathers**

- ▷ **Sherrington:**

- Leave hotel. Turn left and walk towards Metropolitan Cathedral. Follow Mt Pleasant round to the left. Cross Brownlow Hill by the University Square (Blackwell's bookshop) and walk along the pedestrianized area by the Electrical Engineering building and the Harold Cohen Library. Continue straight on along Ashton St. Sherrington is on the right at the end. (10 mins)

- ▷ **Surface Science Research Centre:**

- Leave hotel. Turn left and walk towards Metropolitan Cathedral. Cross Mt Pleasant and follow Oxford Street. Ahead of you there is a 'bridge' across the road. Look left just before the bridge and you will see the Surface Science Research Centre entrance. (5 mins)

- **Cocoon International Inn**

- ▷ **Sherrington:**

- Leave hotel and turn right, then right again along Maryland St. At the end turn left along Hope St. Continue straight on to cross the road at the traffic lights and bear right along Mt Pleasant. Cross Brownlow Hill by the University Square (Blackwell's bookshop) and walk along the pedestrianized area by the Electrical Engineering building and the Harold Cohen Library. Continue straight on along Ashton St. Sherrington is on the right at the end. (10 mins)

- ▷ **Surface Science Research Centre:**

- Leave hotel and turn right, then right again along Maryland St. At the end turn left along Hope St. Continue straight on to turn right along Oxford St at the traffic lights. Ahead of you there is a 'bridge' across the road. Look left just before the bridge and you will see the Surface Science Research Centre entrance. (5 mins)

- **Hope Street Hotel**

- ▷ **Sherrington:**

- Turn left along Hope St. Continue straight on to cross the road at the traffic lights, continue along Hope Street, cross another set of lights and bear right along Mt Pleasant. Cross Brownlow Hill by the University Square (Blackwell's bookshop) and walk along the pedestrianized area by the Electrical Engineering building and the Harold Cohen Library. Continue straight on along Ashton St. Sherrington is on the right at the end. (10 mins)

—▷ Surface Science Research Centre:

Turn left along Hope St. Continue straight on to cross the road at the traffic lights, continue along Hope Street, cross another set of lights and turn right along Oxford St. Ahead of you there is a 'bridge' across the road. Look left just before the bridge and you will see the Surface Science Research Centre entrance. (5 mins)

• Adelphi**—▷ Sherrington:**

Leave hotel and turn left then left again to walk up the hill (called Brownlow Hill). After about 5 mins, you will see the University Square (Blackwell's bookshop). Turn left and walk along the pedestrianized area by the Electrical Engineering building and the Harold Cohen Library. Continue straight on along Ashton St. Sherrington is on the right at the end. (10 mins)

—▷ Surface Science Research Centre:

Leave hotel and turn left, then cross the road and walk up the hill (Mt Pleasant). When you reach the Metropolitan Cathedral, cross Mt Pleasant and follow Oxford Street. Ahead of you there is a 'bridge' across the road. Look left just before the bridge and you will see the Surface Science Research Centre entrance. (10 mins)

• Lime Street Holiday Inn**—▷ Sherrington:**

Leave hotel and walk along Lime Street with St George's Hall on your left and the Station and North Western Hall on your right. Turn right at the end up London Rd. Stay on the right hand side of the road and walk up the hill. After 5-10 mins, you will begin to see University buildings, such as the Tropical Medicine school. When you reach Ashton St, you will see the Sherrington building. (15 mins)

—▷ Surface Science Research Centre:

Leave hotel. Cross Lime Street and walk along Renshaw St (to the right). When you reach the Adelphi, cross the road and walk up the hill (Mt Pleasant). When you reach the Metropolitan Cathedral, cross Mt Pleasant and follow Oxford Street. Ahead of you there is a 'bridge' across the road. Look left just before the bridge and you will see the Surface Science Research Centre entrance. (15 mins)

• Marriott**—▷ Sherrington, Surface Science Research Centre:**

Leave the hotel and walk up St John's Lane and St George's Place to the Lime Street Holiday Inn and follow instructions from there. (15 mins)

• The Liner**—▷ Sherrington:**

Leave the hotel and walk up the hill (Lord Nelson St) to Seymour St. Turn left and then turn right at the traffic lights to walk up London Rd. After 5 mins, you should see the School of Tropical Medicine on the right and the Dental Hospital on the left. Continue walking and you will see the Sherrington on Ashton St on the right. (5 mins)

—▷ **Surface Science Research Centre:**

Leave the hotel and walk up the hill (Lord Nelson St) to Seymour St. Turn right and continue along Seymour St and then Russell St and then Clarence St and then turn left onto Mt Pleasant. Walk up the hill towards Metropolitan Cathedral. Cross Mt Pleasant and follow Oxford Street. Ahead of you there is a 'bridge' across the road. Look left just before the bridge and you will see the Surface Science Research Centre entrance. (15 mins)

• **Eleanor Rigby Hotel**

—▷ **Sherrington, Surface Science Research Centre:**

Turn left along Stanley Street, then right along Victoria Street. Before the roundabout turn right up St John's Lane to the Marriott, then follow instructions from there. (20 mins)

• **Premier Inn**

—▷ **Sherrington, Surface Science Research Centre:**

Turn left along Vernon St, then left again along Dale Street. Cross the road and walk along Crosshall St to Victoria St. From here follow instructions per the Eleanor Rigby Hotel. (20 mins)

• **Jury's Inn**

—▷ **Sherrington, Surface Science Research Centre:**

Walk out of the Docks to find yourself on Wapping. Turn left and then right along Liver St. Follow the road round to the left (Paradise St) to Duke St. Walk up Duke St to the Anglican Cathedral (10 mins). Turn left along Hope St and walk along it to the Hope St Hotel (opposite the Philharmonic Hall) and follow instructions from there. (25 mins)

• **Express by Holiday Inn**

—▷ **Sherrington, Surface Science Research Centre:**

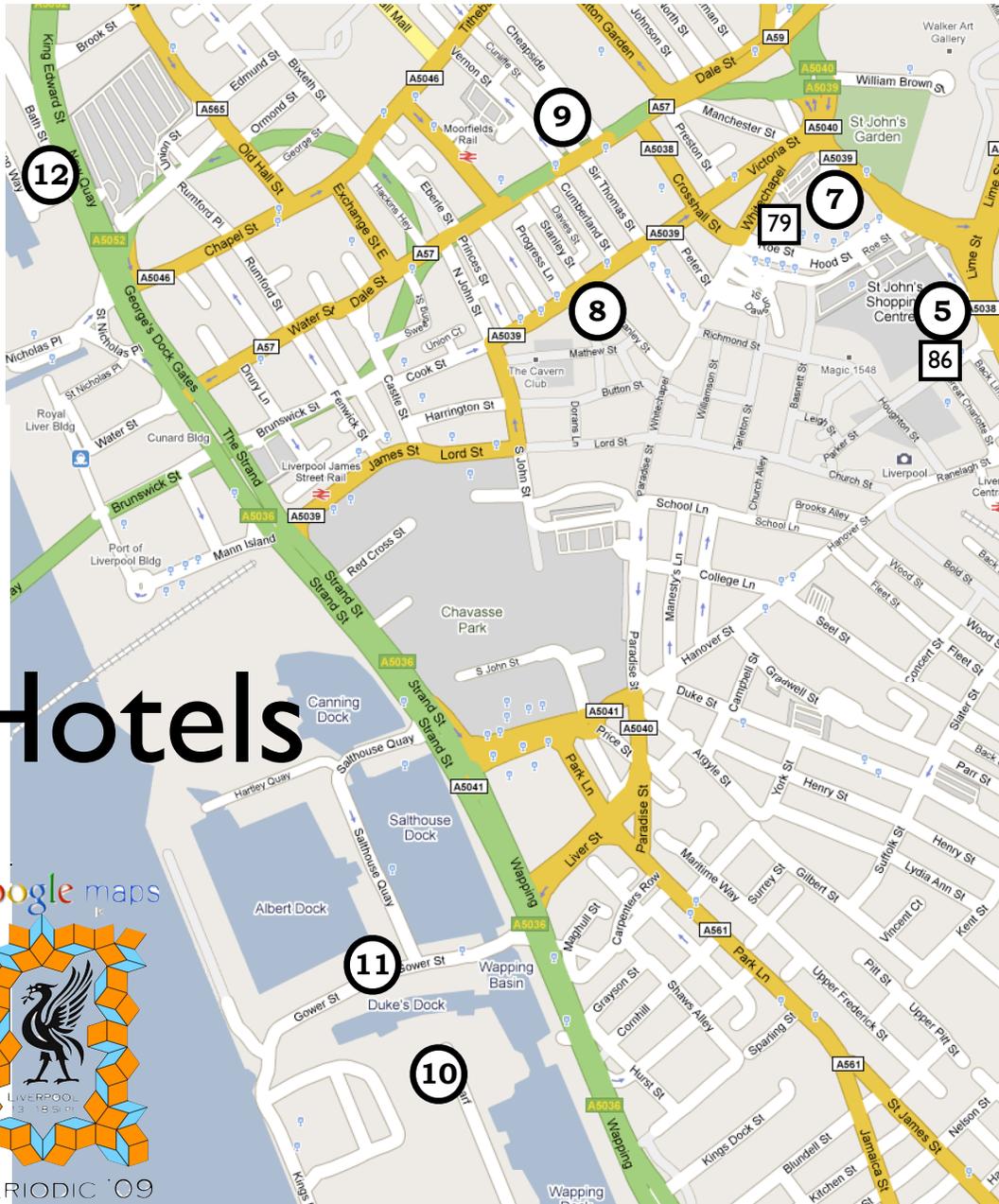
As for Jury's Inn.

• **Malmaison**

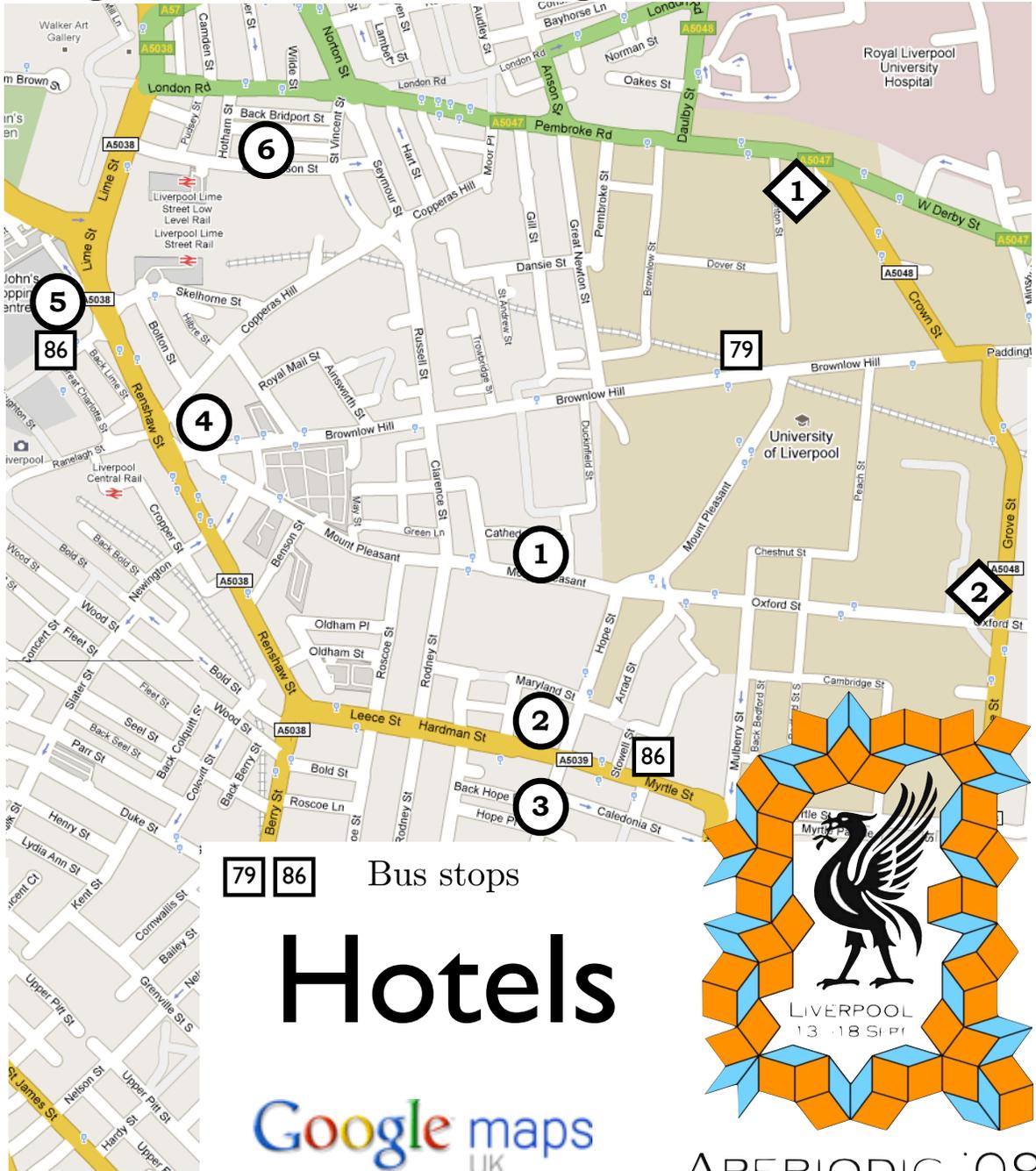
—▷ **Sherrington, Surface Science Research Centre:**

Walk out of the Docks to find yourself on New Quay. Cross the road at a crossing, and walk towards the Liver Building. When you reach it, turn left along Water St. Continue past the Town Hall at the top of Water St and up Dale St to Crosshall St. From here follow instructions as per the Premier Inn. (25 mins)

- | | |
|----------------------------------|----------------------------------|
| 79 86 Bus stops | 9 Premier Inn |
| 5 Lime Street Holiday Inn | 10 Jury's Inn |
| 7 Marriott | 11 Express by Holiday Inn |
| 8 Eleanor Rigby Hotel | 12 Malmaison |



- | | |
|----------------------------|--|
| ① Feathers | ◇ 1 Sherrington Building and Madison's |
| ② Cocoon International Inn | ◇ 2 Surface Science Research Centre |
| ③ Hope Street Hotel | ⑥ The Liner |
| ④ Adelphi | |



79 86 Bus stops

Hotels

Google maps UK



APERIODIC '09

7 Restaurant suggestions

- **Mr Chilli**

Authentic Chinese Szechuan restaurant. £10-£20 per person.

48 Mount Pleasant, 0151 708 8484

- **Maharajah**

The food, typical of India's coastal Kerala region, is light (everything is cooked in water, not oil), sensitively seasoned, with fresh, zingy herbs and spices, and full of long, lip-smacking flavours. (www.guardian.co.uk)

34-36 London Road, +44 (0)151 709 2006; £10-£25 per person.

- **Eureka**

Popular Greek restaurant. £10 per person lunch, £20 per person dinner.

7 Myrtle Parade, 0151 709 7225

- **Ego**

Popular Mediterranean restaurant in a nice location by the Philharmonic Hall. £10-£20 per person.

Hope Street, 0151 706 0707

- **Delifonseca**

A deli-cafe. Pick up posh snacks in the deli (gourmet sandwiches, Pipers' outstanding crisps, Mawson's traditional drinks), or head upstairs to the attractive casual diner.

Mains £6.45 to £12.75. 12 Stanley Street, +44 (0)151 255 0808

- **The Egg Cafe**

Vegetarian. Specials might include goulash or chilli, alongside fat quiches, good salads and interesting soups. . Vegan available. (www.guardian.co.uk)

Specials £5.95; cheese-on-toast £3.70. Top Floor. Newington Buildings, 16-18, Newington, +44 (0)151 707 2755

- **Tokyou**

The menu is mainly Cantonese, Japanese and Malaysian. It's conveniently open 12.30pm-11.30pm daily.

Mains £3.80 to £6.20. 7 Berry Street, +44 (0)151 445 1023

- **The Side Door**

High quality varied cuisine located in one of Hope Street's handsome Georgian terraces, halfway between the Everyman theatre and the Philharmonic Hall.

Theatre menu, two-courses £15.95; three courses £17.95. 29a Hope Street, +44 (0)151 707 7888

- **Kimos**

Busy halal cafe does a good line in the obvious filled spuds, burgers, pizza and panini. Much more interesting, however, are its Mediterranean, Middle Eastern and north African dishes.

Breakfasts £3.90. 38 Mount Pleasant, +44 (0)151 707 8288

- **Tate Cafe**

Simple dishes like hot pot, chorizo stew or fish cakes, with an emphasis on premium regional ingredients like Rhug Estate steak and Mrs Kirkham's Lancashire cheese.

Light lunches £5.50; mains £7.55. Albert Dock, +44 (0)151 702 7581

- **Baltic Fleet**

The last surviving sailor's pub on Liverpool's dockside. The Baltic is also a brew-pub renowned for its own Wapping beers.

Mains £3.95 to £6.95. 33a Wapping, +44 (0)151 709 3116

- **The Quarter**

Cheap, reliable homemade pasta dishes and above-average, stone-baked pizzas.

Pasta £5.99 to £8.50; pizza £4.85 to £6.99. 7 Falkner Street, +44 (0)151 707 1965

⑤ Delifonseca

⑩ Tate Cafe

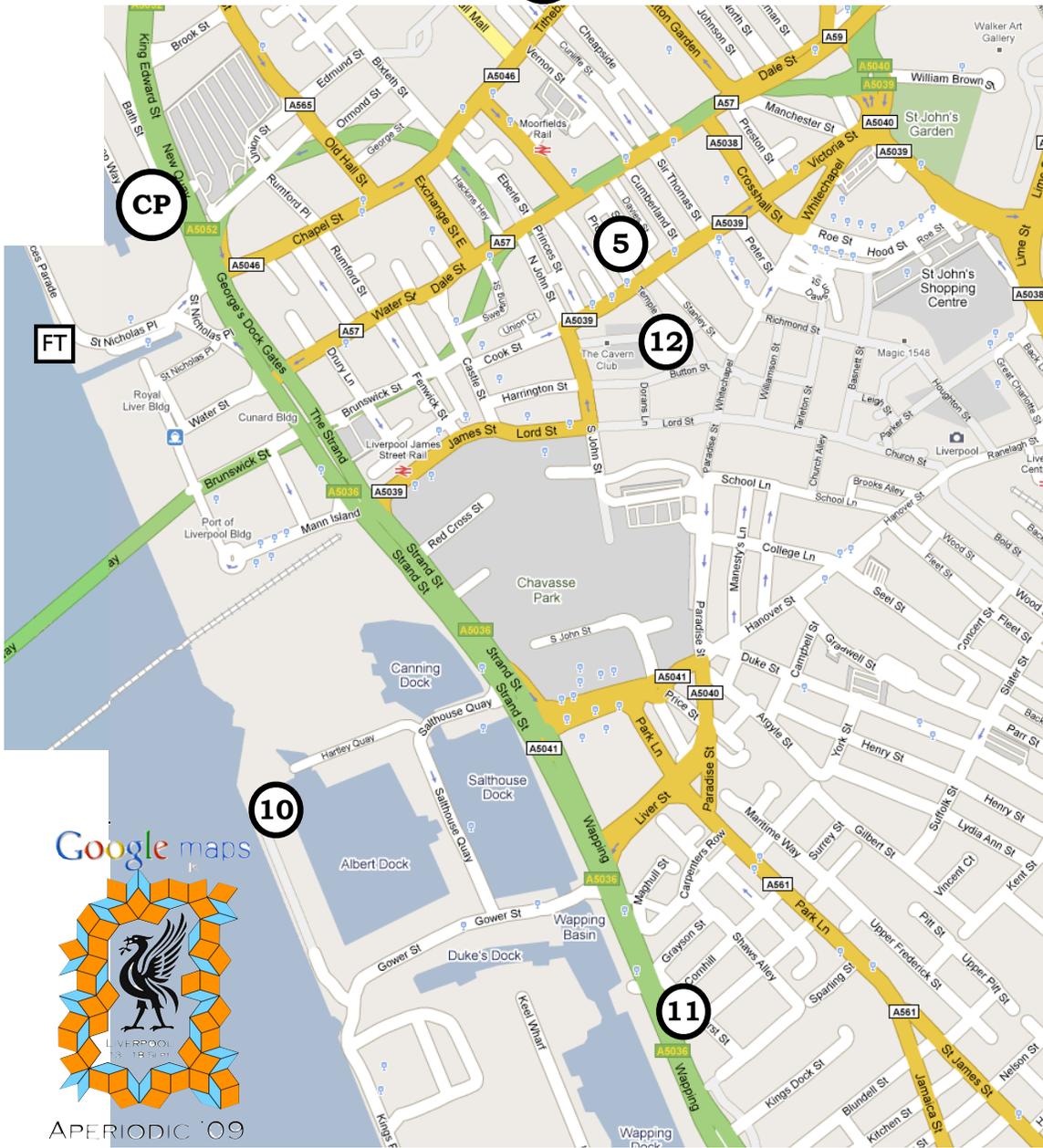
⑪ Baltic Fleet

⑫ The Quarter

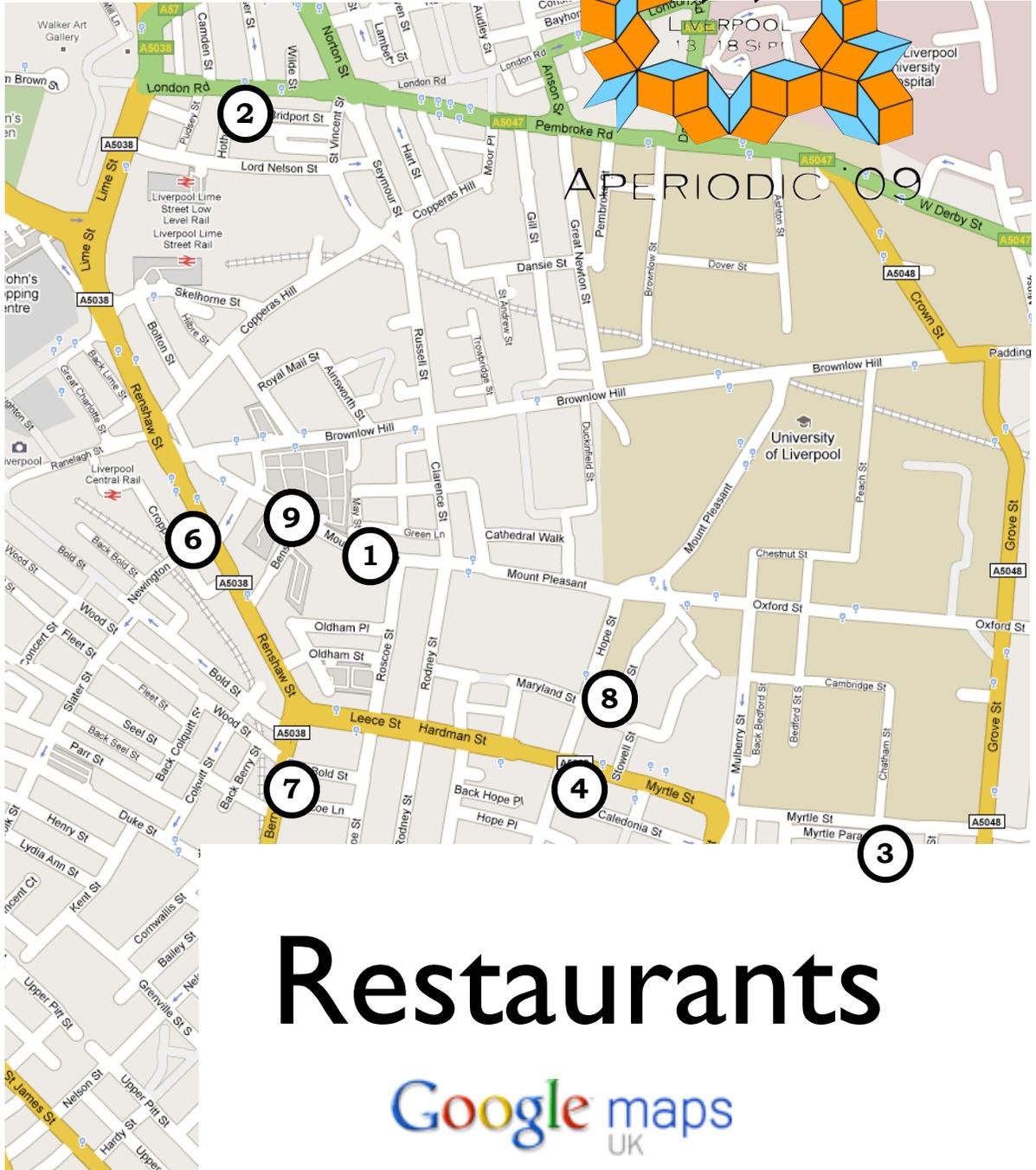
FT Ferry terminal

CP Crowne Plaza
(Conference Dinner venue)

Restaurants



- | | |
|-------------|-----------------|
| ① Mr Chilli | ⑥ The Egg Cafe |
| ② Maharajah | ⑦ Tokyou |
| ③ Eureka | ⑧ The Side Door |
| ④ Ego | ⑨ Kimos |



Restaurants



8 About Liverpool

Founded in 1207, Liverpool has a population of 435,000 (815,000 including suburban areas). Referred to as 'Scousers' (in reference to a local delicacy called 'scouse'), they are a diverse population with a wide range of cultures and religions drawn from all over the world, owing to Liverpool's importance as a port. The city is home to the oldest Black community in Britain, dating from the 1700s and the oldest Chinese community in Europe – the first residents of the city's Chinatown arrived as seamen in the 1800s.

Figure 1: Liverpool and the Mersey in 1680



Figure 2: The Chinese Gate in Liverpool

This importance of the ports at Liverpool has historically led to the city being considered 'the second city of the Empire' (Disraeli), 'the New York of Europe' (Illustrated London News, 1885) and the 'pool of life' (Jung). However, following severe bombing in the Second World War and hurried reconstruction efforts that were then rendered obsolete by modernization of the shipping system, trade went into a sharp decline starting in the 1970s. Today the city is back on an upward trend, being named 'European Capital of Culture' in 2008.

Being located in the northwest of England, the Gulf Stream maintains a mild climate, though rainfall is high, with an occurrence on 282 days out of the year. However, this year we have so far experienced a very pleasant summer, with temperatures as high as 28 degrees Celsius.

8.1 Landmarks

The extreme wealth of Liverpool during its heyday (at some times in the 19th century, the city was more wealthy than London) means that some of the finest architecture in Britain may be found here. This architecture exists in a considerable variety of styles, due to the history of the city, ranging from 18th century Tudor to modern day contemporary architecture.

There are over 2,500 listed buildings in Liverpool, more than any other city apart from London. The city also has a greater number of public sculptures than any location apart from Westminster and more Georgian houses than the city of Bath.

Delegates who manage to go on the ferry trip planned as part of the mid-conference activities, will have the Stanley Dock Tobacco Warehouse building pointed out to them. This building at the time of its construction was the largest building in the world. Even today, it stands as the largest brickwork building in the world.

Liverpool has a very recognizable skyline, which until recently was dominated by the so-called Three Graces: the Liver Building, the Cunard Building and the Port of Liverpool Building, all of which stand on the Pier Head, from which ferries across to the Wirral Peninsula, the Isle of Man and Ireland depart. Over the past few years, as part of the Liverpool redevelopment scheme, some tower blocks have been constructed that dwarf the traditional buildings of the Mersey waterfront.

Figure 3: The skyline of Liverpool (courtesy www.PeteCarr.net). The three central buildings are the Three Graces.



Figure 4: Clockwise from top left: Liverpool Town Hall, St George's Hall, Metropolitan Cathedral, Anglican Cathedral

The Commercial District, centred around Castle Street and Dale Street, has some of Liverpool's finest buildings. Liverpool Town Hall, situated at the junction of these two streets, is one of the most extravagantly decorated buildings in Britain and is considered to be the finest Georgian building in the city. Amongst the other noted buildings in the area are the Tower Buildings, Albion House (the former White Star Line headquarters), the Municipal Buildings and Oriel Chambers, which is considered to be one of the earliest Modernist style buildings ever built.

The Cultural Quarter is home to the William Brown Library, Walker Art Gallery, Picton Reading Rooms and World Museum Liverpool. The area is dominated by neo-classical architecture, of which the most prominent (and the first building you see on leaving Liverpool Lime Street Station) is St George's Hall, widely regarded to be the best example of a neo-classical building anywhere in Europe.

Liverpool is also noted for having two huge cathedrals. Joined by the optimistically-named Hope Street, the cathedrals dominate their respective areas. The Anglican Cathedral is the largest cathedral in Britain, and the fifth largest in the world. Designed and built in Gothic style by Sir Giles Gilbert Scott, it is regarded as one of the greatest buildings to have been constructed during the 20th century and was described by former British Poet Laureate, John Betjeman, as 'one of the great buildings of the world. The Metropolitan Cathedral was constructed between 1962 and 1967 and is noted as one of the first Cathedrals to break the traditional longitudinal design.

The Metropolitan Cathedral is located next to the University Campus. It has a conical shape, topped by a huge stained-glass lantern that is the largest stained glass panel in the world. When construction on the Anglican Cathedral began, plans for the Metropolitan cathedral were proposed, just the atrium of which could have held the Victoria Building (the large red building which is the original building of Liverpool Engineering College, the first building of the University). However, this plan proved exorbitantly expensive, and just the crypt of the original design was built. The cathedral that stands now was constructed between 1962 and 1967 and is the result of a architectural competition to build a cathedral for under 1 million won by Sir Frederick Gibberd.

8.2 Culture and sport

8.2.1 Music and poetry



Liverpool was the centre in the 1960s of Merseybeat and since then has been home to a music scene. Many musicians, including Michael Jackson consider the city to be the spiritual home of contemporary pop music due to success of The Beatles, about whom we will learn on Wednesday's trip to The Beatles Story. The city is also home to the Royal Liverpool Philharmonic Orchestra, headquartered in the Philharmonic Hall (where University of Liverpool degrees are conferred), and to a youth orchestra. Max Bruch was one of numerous notable conductors of the RLPO, and dedicated his Kol Nidre to the Jewish community in the city.

Sir Edward Elgar dedicated his famous Pomp and Circumstance No.1, to the Liverpool Orchestral Society, and the piece had its first performance in the city in 1901. Among Liverpool's curiosities, the Austrian emigré Fritz Spiegl is notable. He not only became a world expert on the etymology of Scouse, but composed the music to Z-cars and the Radio 4 UK Theme.

During the late 1960s the city became well-known for the Liverpool poets, who include Roger McGough and the late Adrian Henri. An anthology of poems, *The Mersey Sound*, written by Henri, McGough and Brian Patten, has sold over 500,000 copies since first being published in 1967.

8.2.2 Theatre

Liverpool also has a history of performing arts, reflected in its annual theatrical highlight The Liverpool Shakespeare Festival which takes place inside Liverpool Cathedral and in the adjacent historic St James' Gardens every summer, and by the number of theatres in the city. These include the Empire, Everyman, Liverpool Playhouse, Neptune, Royal Court and the Unity Theatre. The Everyman Theatre, Unity Theatre and Playhouse Theatre all run their own theatre companies.



8.2.3 Visual arts



Liverpool has more galleries and national museums than any other city in the United Kingdom apart from London. National Museums Liverpool is the only English national collection based wholly outside London. The Tate Liverpool gallery houses the modern art collection of the Tate in the North of England and was, until the opening of Tate Modern, the largest exhibition space dedicated to modern art in the United Kingdom. The FACT centre hosts touring multimedia exhibitions, whilst the Walker Art Gallery houses an extensive collection of Pre-Raphaelites. Sudley House contains another major collection of pre 20th century art and the number of galleries continues to expand: Ceri Hand Gallery opened in 2008, exhibiting primarily contemporary art, and Liverpool University's Victoria Building was re-opened as a public art gallery and museum to display the University's artwork and historical collections which include the second-largest display of art by Audubon outside the US. Artists have also come from the city, including painter George Stubbs who was born in Liverpool in 1724.

8.2.4 Football

Liverpool is home to two Premier League football clubs - Liverpool F.C. and Everton. Liverpool is the only English city to have staged top division football every single season since the formation of the Football League in 1888, and both of the city's clubs play in high-capacity stadiums.

Liverpool F.C. are the most successful team in English football, having won 18 league titles, seven FA Cups, seven League Cups, five European Cups and three UEFA Cups. They formed in 1892 and have spent their entire history at the Anfield stadium which they occupied on their formation; it had previously been home to Everton.

Everton are the older of Liverpool's two professional football clubs. They were founded in 1878



and have played at Goodison Park since 1892, when they relocated from the Anfield stadium that was taken over by the new Liverpool club. Everton have been league champions nine times, FA Cup winners five times and European Cup Winners' Cup winners once.

10 Session Overview

Sunday 13 September

Session I

Chair: H.R. Sharma

T-01	14:30	E. Abe	Microscopic view of quasicrystal symmetry
T-02	15:30	A. Beni	New complex metallic alloys for industrial applications: Tribological, adhesion and corrosion resistance properties
T-02	16:30	G. Chapuis	Introductory tutorials on incommensurate and composite crystals

Monday 14 September

Session I

Chair: A.P. Tsai

I-01	09:20	H. Takakura	Atomic structure of P-type icosahedral quasicrystals from a unified viewpoint
O-01	10:00	Y. Ishii	Electronic structures and stability of Ag-In-Ca surfaces
O-02	10:20	C.P. Gómez	Chemical and short-range order in RE-Mg-Cd quasicrystal approximants

Session II

Chair: J.M. Perez-Mato

I-02	11:10	J.L. Ribeiro	Incommensurate magnetism and ferroelectricity in rare-earth manganites
O-03	11:50	J.B. Claridge	Incommensurate Bismuth based perovskites; $\text{Bi}_2\text{Mn}_{4/3}\text{Ni}_{2/3}\text{O}_6$
O-04	12:10	R.L. Withers	A careful phase analysis and TEM investigation of the incommensurately modulated, magneto-ferroelectric $(\text{Bi}_{1-x}\text{M}^{\text{II}})\text{Fe}^{\text{III}}\text{O}_{3-x/2}$ ($M = \text{Ca}$ and Sr) solid solutions
O-05	12:30	Th. Weber	The disordered structure of the mineral theoparacelsite

Session III

Chair: M. Shimoda

I-03	14:00	J. Ledieu	Adsorption studies on quasicrystal and approximant surfaces: a comparison
O-06	14:40	M. Krajčí	Structural model of the quasiperiodic Pb monolayer deposited on the fivefold i-Al-Pd-Mn surface
O-07	15:00	S. Olsson	Formation of $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$ quasicrystalline thin films by annealing of sputtered Al-Cu-Fe multilayers
O-08	15:20	H.R. Sharma	Surface and thin film growth studies on icosahedral Ag-In-Yb quasicrystal and related crystals

Session IV

Chair: G. Chapuis

I-04	16:10	J.M. Perez-Mato	Modes vs. modulations: the use of symmetry-adapted modes in the analysis of commensurate modulated structures compared with the superspace method
O-09	16:50	V.F. Degtyareva	Electronic origin of the incommensurate modulation in the structure of phosphorus IV
O-10	17:10	A. Ustinov	Diffraction effects due to modulation of orthorhombic crystals by aperiodically arranged twin boundaries

Tuesday 15 September**Session I****Chair: R.L. Withers**

- I-05 09:00 A. Arakcheeva Beyond modulated structures: contribution of superspace to structure — property investigations
- O-11 09:40 J. Hadermann Generalized superspace description of tetrahedral chain order in brownmillerite type structures
- O-12 10:00 O. Degtyareva Modulated superstructure of β -brass CuZn compressed to 90 GPa
- O-13 10:20 O. Pérez Revisiting tungsten phosphate bronzes using the superspace formalism

Session II**Chair: N.K. Mukhopadhyay**

- I-06 11:10 C. Ecolivet Hidden degrees of freedom in composite aperiodic crystals
- O-14 11:50 H. Euchner Lattice dynamics in complex metallic alloys – vibrational properties of $Zn_{11}Mg_2$
- O-15 12:10 J. Wolny Simple model of Mg_2Al_3 : β and β' phases
- O-16 12:30 T. Yamada Low-temperature phase transition of a Zn_6Sc 1/1 cubic approximant

Session III**Chair: S.I. Ben-Abraham**

- I-07 14:00 M. Baake Surprises in aperiodic diffraction
- O-17 14:40 N. Fujita Order and disorder in ternary decagonal tilings
- O-18 15:00 A. Chatzopoulos The hydrodynamic structure factor of quasicrystals
- O-19 15:20 A. Yamamoto Theory of short-range order magnetic diffuse scattering in quasicrystals and application to random phason flips in the Penrose pattern

Public Lecture: Prof. Sir Roger Penrose (16:15)**Chair: R. McGrath****Poster Session (17:30)****Wednesday 16 September****Session I****Chair: S. van Smaalen**

- I-08 09:00 A.M. Abakumov Modulated structures of mixed ionic conductors $A_4B_6O_{12+2\alpha}$ ($A = Sr, Ba, B = Fe, In, Mg$)
- O-20 09:40 L. Palatinus A general origin-independent space-group identifier applicable to space groups in arbitrary dimensions
- I-09 10:00 M. Dušek Advances in solution of modulated structures reflected by Jana system

Session II**Chair: J. Ledieu**

- I-10 11:10 B. Ünal Terminations, adsorption sites, and metal nano island nucleation and growth on *i*-Al-Pd-Mn quasicrystal surfaces
- O-21 11:50 A.K. Shukla Quantum size effects in the thin metal films grown on complex metallic alloy surfaces
- O-22 12:10 D. Gratias About the chemistry of the termination 5f planes in surface studies of *i*-AlPdMn
- O-23 12:30 M. Shimoda STM Studies of high symmetry surfaces of *i*-In-Ag-Yb quasicrystals

Thursday 17 September**Session I****Chair: W. Theis**

- I-11 09:00 C. Bechinger Geometrical constraints for the formation of 7-fold axial symmetries
- O-24 09:40 M. Schmiedeberg Colloidal particles on substrates with decagonal symmetry
- O-25 10:00 M. Engel Spontaneous formation of a dense aperiodic crystal from hard tetrahedra
- O-26 10:20 R. Lifshitz Stability of quasicrystals composed of soft isotropic particles

Session II**Chair: M. Baake**

- I-12 11:10 M. Loquias Recent developments in the mathematics of grain boundaries
- O-27 11:50 R. Lück Colour groups in tilings with singularities
- O-28 12:10 E.Y. Vedmedenko In search of magnetic long-range order on quasiperiodic tilings
- O-29 12:30 N.E. Kaputkina Aperiodic sequences of quantum dots in external magnetic and electric fields

Session III**Chair: M. de Boissieu**

- O-30 14:00 H. Abe Atomic short-range and medium-range order in Al-Ni-Co decagonal quasicrystals
- O-31 14:20 S. Deloudi Modeling of decagonal quasicrystals
- O-32 14:40 M. Inukai Spectroscopic study on chemical ordering of transition metals in decagonal Al-Co-Ni and Al-Co-Cu quasicrystals
- O-33 15:00 Y. Miyazaki Structure of B-Ti-Ru decagonal approximant crystals
- O-34 15:20 A. Strutz Solution of the average structure of basic Co-rich decagonal Al-Ni-Co based on a five-dimensional model

Science in Fiction: Ann Lingard (16:15)**Chair: U. Grimm****Poster Session (17:30)****Friday 18 September****Session I****Chair: J. Hadermann**

- I-13 09:00 A. Schönleber Phase transitions and modulated structures of Λ -Co(sepulchrates)-trinitrate at low temperatures
- O-35 09:40 J. Roth Quasicrystals of higher irrationality
- O-36 10:00 Ph. Schaub Local disorder in decagonal Al-Cu-Co quasicrystals explored by the three-dimensional pair distribution function
- O-37 10:20 K. Pussi The uniaxially aperiodic structure of a thin Cu film on 5-fold *i*-Al-Pd-Mn

Session II**Chairs: R. McGrath & U. Grimm**

- O-38 11:10 N.K. Mukhopadhyay Evolution and structural transition of quasicrystalline phases in Al-Fe-Cu-Cr and Al-Fe-Cu-Mn alloys during high energy ball milling
- O-39 11:30 K. Nishimoto Low-temperature TEM observations of Cd_6M (M=Sr, Pr, Nd and Sm) approximants
- O-40 11:50 J. Ivkov Hall effect of the Y-Al-Ni-Co and *o*- $\text{Al}_{13}\text{Co}_4$ decagonal approximants

11 Abstracts

11.1 Sunday 13 September

14:30

Tutorial T-01

Title: Microscopic view of quasicrystal symmetry

Author: E. ABE

Address: Department of Materials Science & Engineering, The University of Tokyo, 113-8656, Japan

Abstract: Quasicrystals represent aperiodically ordered form of solids with symmetries long thought forbidden in nature. Since their discovery, the fundamental key question has been "Where are the atoms?" For the last decade major strides have been made in determining atomic structure of decagonal quasicrystals, largely by direct imaging using scanning transmission electron microscopy. The picture that has been emerging from the recent microscopy studies is that the structure of the best-ordered decagonal compounds appears to be a realization of an ideal Penrose tiling, a planar tiling composed of two different tiles with matching rules. Through a direct, real-space imaging of the decagonal structure at a sub-Angstrom scale, I will further focus on this issue with a more strict sense by describing how much the best-ordered quasicrystalline compounds can be close to a perfect Penrose structure, including slight differences of local atomic configurations in terms of vertex symmetry in the Penrose tiling. I will also describe characteristic localized-distributions of point defects that even exist in the best-ordered quasicrystalline specimen, an occurrence of which can be reasonably explained as being due to a phason-degree of freedom.

15:30

Tutorial T-02

Title: New complex metallic alloys for industrial applications: Tribological, adhesion and corrosion resistance properties

Authors: ●A. BENI, P. SCHMUTZ

Address: Empa, Swiss Federal Laboratories for Materials Testing and Research, CH-8600 Dübendorf, Switzerland

Abstract: Complex Metallic Alloys (CMA) are alloys which belong to the family of intermetallics and are characterised by very complex structures, with very large unit cells containing up to thousands of atoms[1]. Those systems exhibit several unusual properties, like very low electrical and heat conductivity which are ascribed to the presence of a pseudo-gap at the Fermi level. This last phenomenon is also thought to determine the peculiar surface properties found on Al based CMA, like low friction coefficient and low wettability, and have an influence on oxide properties. In addition to that, various CMA ternary Al-alloys, especially the ones belonging to the Al-Cr-Fe family, have been found to be highly corrosion resistant in aqueous media, with a performance that is significantly enhanced, if compared to the one of the single pure elements contained in the alloy[2].

Thanks to these outstanding characteristics, promising industrial applications can be envisaged for those materials if the properties measured on model samples can be reproduced on industrially relevant components.

In the talk, an overview of the most attractive properties of CMA and quasicrystalline materials related to industrial applications will be reported, with an extensive introduction on the techniques used and with a presentation of the latest results, taken both from a literature survey and from the experimental work of the authors.

[1] V. Fournée, M.-G. Barthés-Labrousse, J.-M. Dubois, *Solid State Phenomena* **138** (2008) 407.

[2] D. Veys, C. Rapin, X. Li, L. Aranda, V. Fournée, J.M. Dubois, *J. Non-Cryst. Solids* **347** (2004) 1.

16:30**Tutorial T-03****Title:** Introductory tutorials on incommensurate and composite crystals**Author:** G. CHAPUIS**Address:** Laboratory of crystallography, École Polytechnique Fédérale de lausanne (EPFL), BSP/Cubotron, 1015 Lausanne, Switzerland**Abstract:** Incommensurate and composite crystals are part of a more general class of compounds currently called aperiodic crystals. Aperiodic crystals are characterised by discrete diffraction patterns whose intensities cannot be indexed with the conventional three indices but require additional ones. They occur in almost every type of solids including organic and inorganic compounds, minerals, metals and alloys and even macromolecules. It is convenient to describe their structures in superspace, a conceptual environment in $(3+n)D$ with $1 \leq n \leq 3$, in which three-dimensional aperiodic crystals recover their periodicity. The inconveniences of adding extra dimensions is negligible with regards to all the advantages resulting from the properties of periodicity (diffraction phenomena, Fourier transform, symmetry). Aperiodic structures and in particular incommensurate and composite structures are published regularly in journals dedicated to structural sciences. Numerous softwares exists for the collection and treatment of diffracted intensities by single crystal and powder diffraction and for the resolution of their structures, where the charge flipping algorithm seems to be most successful.

The studies of aperiodic structures has greatly contributed to a better understanding of the physics and chemistry of atomic interactions in crystals. Perhaps the most impressive development concerns the study of modular, polytypes and homologous series of structures. Whereas the relations of their structures and symmetries in 3D is sometimes difficult to identify, it appears that the use of superspace greatly facilitates their description by revealing hidden common denominators and symmetries. This opens also new perspectives in the attempt to correlate the structural with the physical properties of complex materials.

11.2 Monday 14 September**09:20****Invited Talk I-01****Title:** Atomic structure of P-type icosahedral quasicrystals from a unified viewpoint**Author:** H. TAKAKURA**Address:** Division of Applied Physics, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan**Abstract:** We review atomic structure of CdYb and ZnMgHo P-type icosahedral quasicrystals (QC's) based on our six-dimensional models. These QC's (or family of Tsai- and Bergman-type QC's) are explained as structures with different atomic decorations of the same building units: rhombic triacontahedron (RTH), acute rhombohedron (AR) and obtuse rhombohedron (OR). The CdYb QC has ideally simple structure among known icosahedral QC's, since it is a binary structure and the atoms involved in the RTH units are about 94 % of all atoms in the structure. Therefore, there is no ambiguity regarding atomic decoration of the building units within the model. In the case of ZnMgHo P-type QC, several decoration variations, which depend on the local environment, for the OR and AR units exist. What makes the situation more complex is that the QC forms as a ternary alloy. However, approximant crystals provide clues to an understanding of the structure. We also discuss how the present model of ZnMgHo P-type QC can be extended to F-type QC in reference to the recently analyzed ZnMgHf 1/1 approximant crystal [1] that is considered to be an approximant crystal to the corresponding F-type QC.[1] C.P. Gómez *et al.*, *Inorg. Chem.* **47** (2008) 8258.**10:00****Talk O-01****Title:** Electronic structures and stability of Ag-In-Ca surfaces**Authors:** Y. HATORI¹, K. NOZAWA², ●Y. ISHII¹**Addresses:** ¹Department of Physics, Chuo University, Tokyo 112-8551, Japan²Graduate School of Materials Science, University of Hyogo, Hyogo 678-1297, Japan**Abstract:** Quasicrystals (QCs) are long-range ordered materials with rotational symmetry incompatible with translational one. The Fermi energy of QC-related compounds is usually located at a pseudogap in the electronic density of states and hence minimizing the band energy. Such characteristic electronic structures also affect chemical properties of QC surfaces. Extensive studies on clean surfaces of Al-based QCs have shown that Al-rich surfaces are more stable than those with higher concentration of transition elements where surface dangling bonds associated with transition d-states cost larger energy. One may interpret this observation as a consequence of the sp-d hybridization, which is considered important for the pseudogap formation. To study how such selectivity and surface properties are modified for a family of Cd-based QCs, for which the sp-d hybridization is again considered to play an essential role. Since experimental data for Cd-based compounds are not available, we study electronic structures of a slab of Ag-In-Ca cubic approximant. Charge density distributions simulating STM images are calculated for relaxed surface and it is found that Ag and In sites are distinguishable by changing a bias voltage. A role of the sp-d hybridization on surface electronic structures will be discussed.

10:20

Talk O-02

Title: Chemical and short-range order in RE-Mg-Cd quasicrystal approximants

Authors: •C.P. GÓMEZ^{1,2}, A. YAMAMOTO², N. KAMIYAMA³, A.P. TSAI^{2,3}

Addresses: ¹ICYS-MANA ²National Institute for Materials Science ³Institute of Multidisciplinary Research for Advanced Materials, Tohoku University

Abstract: Chemical order has been analyzed in several 1/1 Pr-Mg-Cd Tsai-type quasicrystal approximants with different Mg contents. The average structures have been refined and the single crystal refinements reveal the existence of preferred atomic sites in the structures which are sensitive to chemical substitution by Mg. By comparing several samples with different Mg contents we can detect successively which atomic sites will be most affected as the Mg content increases. Furthermore relatively strong diffuse scattering has been observed in these samples. Refinements on the average structures reveal that interstitial atomic positions responsible for superlattice ordering in other RE-Cd approximants [1, 2] have significant occupancies also in the investigated Pr-Mg-Cd phases. Based on this fact, a model for the short-range order has been developed. Calculated intensities based on this model agree well with experimental measurements. The changes in the correlation length of this short-range order can be directly attributed to the content of Mg in the samples.

[1] C.P. Gómez, S. Lidin, Chem. Eur. J. **10** (2004) 3279.

[2] M. Armbrüster, S. Lidin, J. Alloys Compd. **307** (2000) 141.

11:10

Invited Talk I-02

Title: Incommensurate magnetism and ferroelectricity in rare-earth manganites

Author: J.L. RIBEIRO

Address: Centro de Física, Universidade do Minho, 4710-057 Braga, Portugal

Abstract: The orthorhombic rare-earth manganites RMnO_3 (R=Gd, Tb, Dy) are among the simplest examples of a novel class of frustrated magnets in which an electric polarization is induced by a modulated magnetic order parameter. In this communication, this type of improper ferroelectricity will be analyzed from the point of view of the symmetry. The full magnetic symmetry of the system will be considered and the complete irreducible co-representations of the paramagnetic space group will be used to describe the symmetry of the possible ordered phases induced by commensurate or incommensurate magnetic modulations. The existence of secondary order parameters, such as strain, magnetization, electric polarization or toroidal moment, will be examined in order to elucidate the possible co-existence of different ferroic orders. The temperature-magnetic field phase diagram of TbMnO_3 will be discussed.

11:50

Talk O-03

Title: Incommensurate Bismuth based perovskites; $\text{Bi}_2\text{Mn}_{4/3}\text{Ni}_{2/3}\text{O}_6$

Authors: •J.B. CLARIDGE¹, M.J. ROSSEINSKY¹, H. HUGHES¹, O. PEREZ², D. GREBILLE²

Address: ¹University of Liverpool, Liverpool, UK ²Laboratoire CRISMAT-ENSICAEN, Caen, France

Abstract: Materials in which dielectric and magnetic properties are coupled are of interest for multiple state memory and information storage applications, and fundamentally in terms of the mechanisms for coupling these properties. Single phase materials which display these properties are important as detailed studies of structural response are possible to permit the identification of the underlying mechanisms for this behaviour. In our search for ferromagnetic ferroelectrics based on Bi^{3+} , we have isolated $\text{Bi}_2\text{Mn}_{4/3}\text{Ni}_{2/3}\text{O}_6$. This is a very unusual material as it adopts the perovskite structure with Bi^{3+} on the A site – there has only been one previous example of perovskite stable to ambient pressure synthesis, BiFeO_3 . The material is spin-glass-like with a freezing temperature, T_f , of 35K due to competing exchange interactions on the B site of the perovskite structure and undergoes an incommensurate to commensurate transition above 410K which shows hysteresis. Structurally the material is very interesting – it is very slightly incommensurate, it can be described in terms of the 3+2 dimensional space group $\text{Ibmm}(0-p0,q0)\text{mm.ss}$ ($2ap \times 2ap \times 2ap$; p,q). This modulation is responsible for suppressing the polarisation apparent in single crystal diffraction studies with conventional q-resolution. The modulation can be thought of as arising due to the need to accommodate three distinct cations on the octahedral site and the asymmetric low coordination number environment preferred by Bi^{3+} . Full refinements have been carried out on constant wavelength neutron diffraction data.

12:10

Talk O-04

Title: A careful phase analysis and TEM investigation of the incommensurately modulated, magneto-ferroelectric $(\text{Bi}_{1-x}\text{M}^{\text{II}})\text{Fe}^{\text{III}}\text{O}_{3-x/2}$ ($M = \text{Ca}$ and Sr) solid solutions

Authors: •R.L. WITHERS¹, J. SCHIEMER¹, L. NORÉN¹, Y. LIU¹, L. BOURGEOIS²

Addresses: ¹Research School of Chemistry, Australian National University, Canberra, Australia
²Monash Centre for Electron Microscopy and Department of Materials Engineering, Monash University, Melbourne, Australia

Abstract: A careful phase analysis and TEM investigation of the $(\text{Bi}_{1-x}\text{Ca}_x)\text{Fe}^{\text{III}}\text{O}_{3-x/2}\text{V}_{x/2}$ (V for vacancy), $\sim 0.20 \leq x \leq \sim 0.50$, and $(\text{Bi}_{1-x}\text{Sr}_x)\text{Fe}^{\text{III}}\text{O}_{3-x/2}\text{V}_{x/2}$, $0.2 \leq x \leq 0.67$, perovskite related solid solution fields has been carried out. Both solid solution fields are, in general, (3+1)-d incommensurately modulated with an incommensurate primary modulation wave-vector magnitude that varies systematically with composition. High Resolution (HR)TEM imaging is used to show the presence of at least 6-fold twinning on a sometimes rather fine scale, the fine scale twinning being much more prevalent in the $M = \text{Sr}$ than the $M = \text{Ca}$ system. The (3+1)-d superspace group symmetry is suggested to be $Cmmm(0,1,\gamma)0s0$ or one of the non-centrosymmetric sub-groups thereof. The magnetic and electrical properties of the systems are briefly discussed and a tentative structural model proposed.

12:30

Talk O-05

Title: The disordered structure of the mineral theoparacelsite

Authors: •TH. WEBER¹, D. CHERNYSHOV², R. CERNY³

Addresses: ¹Laboratory of Crystallography, ETH Zurich, Zurich, Switzerland ²Swiss-Norwegian Beamline, ESRF, France ³Laboratory of Crystallography, University of Geneva, Switzerland

Abstract: Theoparacelsite is a rare copper arsenite hydroxide mineral. Due to its close structural relation to the spin-Peierls phase CuGeO_3 and to the anti-ferromagnetic chain compound CuSiO_3 it is expected to show interesting one-dimensional physical properties [1]. Theoparacelsite is disordered and therefore the understanding of the real structure is a key for the understanding of the physical properties. From the average structure it is known that pronounced disorder is found at As sites, which are occupied by 2/3 only. Arsenic occupational disorder is accompanied by distortions in the environment of the As/Void positions and possibly by occupational disorder of oxygen. A low temperature ($T = 15\text{K}$) diffuse scattering data set recorded at the Swiss-Norwegian beamline at ESRF, allowed a detailed investigation of disorder. Though having only four independent atomic sites in the average structure, the diffuse pattern shows a wealth of diffraction features of different dimensionality and strongly varying half-widths. Perpendicular to \mathbf{b}^* diffuse layers are visible between the Bragg layers at $k = m/3$ ($m \neq 3n$), which indicate the presence of a disordered three-fold superstructure along \mathbf{b} . Broad diffuse maxima within these layers are found at incommensurate positions along \mathbf{c}^* . In layers with $k = \text{integer}$, a set of diffuse streaks connects Bragg reflections along \mathbf{c}^* . Beneath the Bragg peaks, narrow diffuse maxima with strongly asymmetric profiles relative to the Bragg positions are observed, indicating presence of a so-called size effect. Details of quantitative Monte Carlo simulations of disorder will be presented.

[1] H.H. Otto, H. Wolfram, Z. Krist. **217** (2002) 431–434.

14:00

Invited Talk I-03

Title: Adsorption studies on quasicrystal and approximant surfaces: a comparison

Authors: •J. LEDIEU¹, R. ADDOU¹, TH. DENIOZOU¹, A.K. SHUKLA¹, E. GAUDRY¹, M.-C. DE WEERD¹, J.-M. DUBOIS¹, V. FOURNÉE¹, M. KRAJČÍ², J. HAFNER³, M. HEGGEN⁴, M. FEUERBACHER⁴, P. GILLE⁵, Y. GRIN⁶, D. WU⁷, T.A. LOGRASSO⁷, R. WIDMER⁸, O. GROENING⁸

Addresses: ¹Institut Jean Lamour (UMR7198 CNRS-Nancy-Université-UPVM), Ecole des Mines, Parc de Saurupt, 54042 Nancy Cedex, France ²Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, SK-84511 Bratislava, Slovak Republic ³Fakultät für Physik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria ⁴Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany ⁵LMU, Department of Earth and Environmental Sciences, Crystallography Section, Theresienstr. 41, D-80333 München, Germany ⁶Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany ⁷Ames Laboratory, Iowa State University, Ames, IA 50011, USA ⁸EMPA, Nanotech @ Surfaces, Feuerwerkerstraße 39, CH-3602 Thun, Switzerland

Abstract: Much of our understanding of condensed matter and surface science is based on studies of periodic crystals. In recent years, this has been extended through the study of quasicrystals and their surfaces, which, although well ordered, are aperiodic. Now, the growth of approximant systems, which are large unit cell complex metallic alloys close in composition to a related quasicrystalline phase, allows the direct comparison of structural and growth phenomena on related periodic and aperiodic surfaces.

In a first part, we will present a detailed investigation of the (100) surface of the orthorhombic Al₁₃Co₄ crystal using experimental tools and *ab initio* electronic structure calculations. Once the surface prepared, the low energy electron diffraction (LEED) patterns indicate that the surface is pseudo-ten-fold symmetric with the lattice parameters consistent with those from the bulk model. Experimental and simulated scanning tunneling microscopy (STM) images reveal that the surface can be described by an incomplete puckered layer, planes present within the bulk model.

In a second part, this complex metallic alloy surface, approximant of the decagonal quasicrystal, has been used as a template for Pb and Cu adsorption. A preferential nucleation site has been identified for Pb adatoms on the Al₁₃Co₄ surface. Further deposition leads to a pseudomorphic Pb monolayer (ML). A similar phenomenon has been observed while dosing Pb adatoms on the Al-Pd-Mn surface and will be discussed here. A pseudomorphic thin film is also obtained after dosing 1 ML of Cu on the Al₁₃Co₄ surface. Above this coverage and at 473K, new surface Al-Cu phases have been observed. The γ -Al₄Cu₉ phase has been identified using LEED and STM. This phase has been previously characterised while dosing Cu on several quasicrystal surfaces.

14:40

Talk O-06

Title: Structural model of the quasiperiodic Pb monolayer deposited on the fivefold i-Al-Pd-Mn surface

Authors: •M. KRAJČÍ^{1,2}, J. HAFNER², J. LEDIEU³, V. FOURNÉE³

Addresses: ¹Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta 9, SK-84511 Bratislava, Slovak Republic ²Fakultät für Physik and Center for Computational Materials Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria ³Institut Jean Lamour (UMR7198 CNRS-Nancy-Université-UPVM), Ecole des Mines, Parc de Saurupt, 54042 Nancy Cedex, France

Abstract: In the previous work [1] a quasiperiodic Pb monolayer on the fivefold i-Al-Pd-Mn surface has been successfully prepared and characterized by the scanning tunneling microscopy (STM) and other experimental techniques. In [2] the initial adsorption of Pb on the five-fold Al-Pd-Mn quasicrystal surface has been investigated both experimentally and by ab-initio calculations. It was found that Pb monolayer nucleates in pentagonal islands dubbed as starfish (SF) clusters. The atomic structure of the SF clusters has been identified and the calculations confirmed their structural stability. In the present contribution we propose a structural model of the quasiperiodic Pb monolayer grown on the fivefold i-Al-Pd-Mn surface at the coverage close to the saturation. The proposed model reproduces the quasiperiodic ordering of the monolayer described by the τ -scaled P1 tiling (τ is the golden mean) seen also in the STM images. The atomic structure and the stability of some regular local features (e.g. the τ -scaled white flower motif) is discussed. The calculated electronic structure reveals that the density of states of the quasiperiodic monolayer exhibits a pseudogap at the Fermi level – in agreement with previous experimental observations.

[1] J. Ledieu *et al.*, Phys. Rev. B **77** (2008) 073409.

[2] J. Ledieu *et al.*, Phys. Rev. B **79** (2009) 165430.

15:00

Talk O-07

Title: Formation of $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$ quasicrystalline thin films by annealing of sputtered Al-Cu-Fe multilayers

Authors: •S. OLSSON, F. ERIKSSON, J. BIRCH, L. HULTMAN

Address: Thin Film Physics, IFM, Linköping University, Linköping, Sweden

Abstract: For many thin film applications, it is desirable to ensure that the substrate temperature does not exceed 500 °C. To produce quasicrystalline thin films on such substrates a low-temperature process needs to be developed. In this work this is investigated with Al-Cu-Fe as a model system.

Multilayered Al-Cu-Fe thin films have been deposited by triple-target unbalanced high vacuum magnetron sputtering onto Al_2O_3 and Si substrates. The multilayer periods are ranging from $L=1$ nm to $L=400$ nm, with nominal layer thicknesses ratios of 7:2:1 to maintain a global chemical composition corresponding to the quasicrystalline phase. The number of periods was varied from $N=1$ to $N=50$ with total film thicknesses between 10 and 400 nm. The composition of the multilayer sequences was verified using energy dispersive X-ray (EDX) analysis. Isothermal annealing was performed on all samples for temperatures up to 800 °C using an in situ high-temperature X-ray diffraction (HT-XRD) furnace. The temperature was increased in steps of 25 to 90 °C and kept for a minimum of 40 min up to 20 h at each step, while X-ray diffraction was continuously recorded.

It was found that when using Si as a substrate a film-substrate reaction occurred at below 400 °C, where Si diffused into the film. This caused a drift in film composition preventing the quasicrystalline phase region to be reached, and the approximant $\text{Al}_{55}\text{Si}_7\text{Cu}_{25.5}\text{Fe}_{12.5}$ together with other crystalline phases was formed in the temperature range 400 to 670 °C.

When annealing the Al-Cu-Fe thin films grown on Al_2O_3 substrates the individual layers first mixed in to several binary AlCu phases (Al_2Cu , AlCu and Al_4Cu_9) and thereafter ternary Al-Cu-Fe phases (e.g. $\text{Al}_7\text{Cu}_2\text{Fe}$) before the $\text{Al}_{62.5}\text{Cu}_{25}\text{Fe}_{12.5}$ icosahedral quasicrystalline phase was formed. The formation temperature of the quasicrystalline phase was between 400 and 490 °C. By keeping the sample at a relatively low temperature of 580 °C the icosahedral phase transformed into the crystalline $\text{Al}_{50}(\text{CuFe})_{50}$ phase due to Al evaporation from the film.

15:20

Talk O-08

Title: Surface and thin film growth studies on icosahedral Ag-In-Yb quasicrystal and related crystals

Authors: •H.R. SHARMA¹, P.J. NUGENT¹, J.A. SMERDON¹, M. SHIMODA², S. OHASHI³, C. CUI³, R. MCGRATH¹, H. TAKAKURA⁴, A.P. TSAI^{2,3}

Addresses: ¹The University of Liverpool, UK ²National Institute for Materials Science, Tsukuba, Japan ³Tohoku University, Sendai, Japan ⁴Hokkaido University, Sapporo, Japan

Abstract: By employing various experimental techniques including scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED) on different high symmetry surfaces of icosahedral Ag-In-Yb quasicrystals and related crystals and with the bulk structure model of the isostructural Cd-Yb, we have determined the surface structure of these new materials. The surfaces are found to be consistent with bulk terminations at the centre of the rhombic triacontahedral clusters (RTH), the building blocks of these materials.

We use these surfaces as templates to grow novel atomic over layers of single elements such as Pb and Sb. Pb forms a bilayer of quasicrystalline structures and after completion of the second layer, five-fold twinned crystalline Pb islands of hexagonal symmetry are formed. These islands exhibit magic heights indicating electron confinement in the islands. The islands are inert for adsorption of C_{60} molecules, while quasicrystalline Pb bilayer and clean surfaces shows strong interaction with the same molecules. Sb also forms a quasicrystalline monolayer, the structure of which is identical to Yb-sites of the substrate. However, at low coverage the structure is inflated by tau. After completion of the monolayer, the film does not show any ordered structure. These results on the new quasicrystal shows promise to extend surface studies beyond Al-based quasicrystals.

16:10**Invited Talk I-04**

Title: Modes vs. modulations: the use of symmetry-adapted modes in the analysis of commensurate modulated structures compared with the superspace method

Author: J.M. PEREZ-MATO

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Abstract: We know from Landau theory that the natural language to deal with displacively distorted structures is the one of modes. Frozen structural distortions can be decomposed into different modes involving collective correlated atomic displacements with symmetries given by irreducible representations (irreps) of the parent space group. This can be useful both for investigating the physical mechanisms that stabilize these phases, and for pure crystallographic purposes. Several computer tools are now available which allow structure refinements using directly collective mode coordinates [1,2]. On the other hand, the superspace formalism is a very efficient method for the analysis and refinement of displacively distorted structures, if described as modulated structures. Both approaches are closely related, being equivalent in simple cases, i.e. each irrep distortion mode corresponds to a specific harmonic in the superspace modulation. However, if the unit cell of the distorted phase is much larger than the parent one, the superspace description is more efficient. On the other hand, for distorted phases with supercells which are only a small multiple of the parent phase and involve modulations along several directions, the mode description is much more convenient. These considerations will be illustrated with several examples.

[1] D. Orobengoa, C. Capillas, M.I. Aroyo, J.M. Perez-Mato, AMPLIMODES: Symmetry mode analysis on the Bilbao Crystallographic Server, *J. Appl. Cryst.* (2009), submitted.

[2] B.J. Campbell, J.S.O. Evans, F. Perselli, H.T. Stokes. *Comp. Comm. Newsletter* **8** (2007) 81.

16:50**Talk O-09**

Title: Electronic origin of the incommensurate modulation in the structure of phosphorus IV

Author: V.F. DEGTYAREVA

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Abstract: Recent high-pressure X-ray diffraction studies revealed unusual structures with incommensurate modulation (IM) in some simple elements [1]. IM structures were found in the elements of group VII (I and Br) and group VI (S, Se and Te). Very recently, an IM structure was found in a light group V element phosphorous in the phase P-IV stable in the pressure range 107-137 GPa [2]. This phase is intermediate between simple cubic and simple hexagonal structures that have atomic coordination equal 6 and 8, respectively. All IM structures were observed when elements become metallic. This implies the importance of the two main contributions into the crystal structure energy: electrostatic (Ewald) and electronic (band structure) energies. The latter can be lowered due to a formation of a Brillouin zone plane and an opening of an energy gap at this plane. Under pressure, the band structure energy part becomes more important leading to a formation of complex low-symmetry structures [3].

We consider configurations of the Brillouin zone and Fermi sphere within a nearly-free-electron model in order to analyze the importance of these configurations for the crystal structure energy [4]. For the phase P-IV with the base-centered orthorhombic structure, oC2, we consider a commensurate approximant with a 11-fold supercell along the c-axis and a modulation wave vector equal 3/11 which is close to the experimentally observed value of 0.267. Atomic shifts due to the modulation result in appearance of satellite reflections and hence in a formation of additional Brillouin zone planes. The stability of this IM structure is attributed to the lowering of the electronic band structure energy due to Brillouin zone Fermi surface interaction. Similar approach is also applied to the IM structure of the group VI elements.

[1] M.I. McMahon, R.J. Nelmes, *Chem. Soc. Rev.* **35** (2006) 943.

[2] H. Fujihisa, Y. Akahama, H. Kawamura *et al.*, *Phys. Rev. Lett.* **98** (2007) 175501.

[3] V.F. Degtyareva, *Physics-Uspekhi* **49** (2006) 369.

[4] V.F. Degtyareva, I.S. Smirnova, *Z. Kristallogr.* **222** (2007) 718.

17:10

Talk O-10

Title: Diffraction effects due to modulation of orthorhombic crystals by aperiodically arranged twin boundaries

Authors: •A. USTINOV^{1,2}, L. OLIKHOVSKA², N. GLAVATSKA², I. GLAVATSKYY²

Addresses: ¹E.O. Paton Electric welding institute of NASU, Kyiv, Ukraine ²G.V. Kurdyumov Institute for metal physics of NASU, Kyiv, Ukraine

Abstract: Phase transformations that take place in cooling of crystals are every so often accompanied by reduction of symmetry of the crystal lattice and occur with formation of twin domains of $\{110\}$, $\langle 1\bar{1}0 \rangle$ system. Such crystals are known to show also the presence of a large number of twin boundaries (TBs) in their low-temperature phases, that the distances between two neighboring TBs can be equal to a few atomic layers. From HREM results, TBs arrangement in the crystal, for the most part, should be considered as a bimodal aperiodic. In the work, the diffraction intensity distributions have been calculated in the kinematic approach for orthorhombic and tetragonal crystals modulated due to a one-modal and bimodal short-range order in the TBs arrangement. Under some conditions of TBs arrangement in the crystals the diffraction pattern shows extra peaks in addition to those related to the primary orthorhombic or tetragonal structure. The extra peaks are irregularly arranged in the identity period of reciprocal crystal lattice. A comparison between the diffraction features resulted from aperiodic TBs arrangement in crystals and the diffraction features caused by static displacement waves in the crystals is made.

Based on the model, the intensity curves were simulated to give a reasonable fit to the diffraction pattern of a layered Ni-Mn-Ga martensite that showed irregular positions of the extra peaks. The results of the work allow the conclusion to be made that the modulated structures, formed in crystals as martensitic transformation occurred, are due to the presence of aperiodic TBs in the crystal. Changes of the diffraction pattern at the change of chemical composition of an alloy can be due to a change in the TBs arrangement in the crystal.

11.3 Tuesday 15 September

09:00

Invited Talk I-05

Title: Beyond modulated structures: contribution of superspace to structure — property investigations

Authors: •A. ARAKCHEEVA, G. CHAPUIS

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Abstract: The example of the $\text{Na}_x\text{Eu}_{2/3-x/3}^{3+}\text{MoO}_4$ ($0 \leq x \leq 0.5$) series of scheelite related compounds (SRCs) illustrates the potential of the application of the superspace symmetry approach to predict and investigate crystal structure - property relations. Six different compositions (with $x = 0.015, 0.134, 0.138, 0.2, 0.236, 0.25$) exhibit different intensity of luminescence in spite of possessing an identical average structure, the unique superspace group, $I2/b(\alpha\beta 0)00$, similar unit cell parameters and atomic positions. Different luminescence intensity induced by the ${}^5\text{D}_0$ - ${}^7\text{F}_2$ transitions of Eu^{3+} ions correlates with different orderings defined by the modulation vector \mathbf{q} and occupation modulation function, which are specific for each member of the family. Some scheelite related compounds (SRCs), such as $\text{KGd}(\text{WO}_4)_2\text{:Nd,Yb}$, $\text{NaBi}(\text{WO}_4)_2$, PbMoO_4 and MWO_4 ($\text{M} = \text{Cd, Pb, Ca}$), are well known in industry; many more of them are the subject of advanced research studies owing to their optical properties, stability and relatively simple preparation. Many SRCs form incommensurately modulated structures, which can only be properly characterized using the superspace symmetry approach. Its application can provide a complete structural characterization of these materials and can also guide the material scientist in its search for an optimum composition to obtain the desired physical properties of SRCs.

Another challenge concerns the interpretation of solid solutions. Apparently, the $\text{Na}_x\text{Eu}_{2/3-x/3}^{3+}\text{MoO}_4$ compounds (at least for $0.134 \leq x \leq 0.25$) can be considered as a typical row of the solid solutions. However, the space group symmetry and unit cell parameters, which are usually specified for solid solutions, can obviously be completed by \mathbf{q} vectors and occupation modulation functions, which are specific for each composition in the common superspace group. The present example leads us to a possible reinterpretation of the solid solution concept by considering the superspace symmetry instead of only the 3D space group symmetry.

09:40

Talk O-11

Title: Generalized superspace description of tetrahedral chain order in brownmillerite type structures

Authors: •J. HADERMANN, H. D'HONDT, A.M. ABAKUMOV

Address: EMAT, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium

Abstract: Brownmillerites $A_2BB'O_5$ (BM) are well-known perovskite based structures with anion-vacancy order that results in chains of $B'O_4$ tetrahedra. Due to cooperative rotations of the tetrahedra, the chains adopt two mirror-related configurations, called L and R. BM have been extensively investigated, however, it appears that for many of the published structures the presence of modulations was overlooked. We defined the structural parameters governing the type of tetrahedral chain order [1], and this led us to re-examine the well-known compound $Sr_2Fe_2O_5$. We found it is actually incommensurately modulated [2]. We expect this to be true also for several other BM structures and have determined how to derive the structure directly from the components of the modulation vector q (easily observable in ED patterns). q has in general two components, one due to the ordered alternation of the L and R chains within the tetrahedral layers (intralayer order), the other due to the displacement of the tetrahedral layers relative to each other (interlayer order). We have expanded the superspace model that exists for the intralayer order [3] in order to also describe possible stacking sequences of the tetrahedral layers, so that both inter- and intralayer chain order can be easily derived from the components of the q -vector [2]. We have investigated the different patterns and made a schematized correspondence between observed ED patterns, space group and structure model, to facilitate these studies in the future.

[1] J. Hadermann *et al.*, *J. Mat. Chem.* **17** (2007) 692–698.

[2] H. D'Hondt *et al.*, *Chem. Mater.* **20** (2008) 7188–7194.

[3] S. Lambert *et al.*, *Chem. Mater.* **14** (2002) 1818–1826.

10:00

Talk O-12

Title: Modulated superstructure of β -brass CuZn compressed to 90 GPa

Authors: •O. DEGTYAREVA¹, V.F. DEGTYAREVA²

Addresses: ¹Centre for Science at Extreme Conditions and School of Physics, University of Edinburgh, Edinburgh, UK ²Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia

Abstract: Cu-Zn is a classic example of an alloy system displaying a sequence of phases along the alloy composition, called Hume-Rothery phases. The crystal structure of these phases is determined by electron concentration (that is the number of valence electrons per atom), and the lowering of the electronic energy is the key factor for their structural stabilization. And because high pressure enhances this stabilization factor, it would be interesting to look at the structural stability of the Hume-Rothery phases on compression. In our recent high-pressure studies [1] we studied the α -, β - and γ -phases of Cu-Zn with the fcc, bcc and complex cubic structures, respectively, in the pressure range up to 50 GPa. We found that the α - and β -phases show a structural distortion at 17 and 37 GPa, respectively, while the γ -phase remained stable up to the maximum pressure reached.

In our present study we look in detail at the structural distortion of the β -phase of CuZn in the pressure range up to 90 GPa, using synchrotron X-ray diffraction. In the diffraction patterns above 40 GPa we observed splitting of the bcc reflections, as well as appearance of weak superstructure reflections. Splitting of the main reflections is explained by a trigonal distortion of bcc, while the additional reflections are due to a positional modulation along the trigonal axis. We analyze the modulated superstructure of the bcc phase of CuZn by looking at the configuration of the Brillouin zone of the bcc and the trigonal structures and their interaction with the Fermi surface using the program BRIZ [2]. This analysis shows an enhancement of the Hume-Rothery mechanism under pressure.

[1] V.F. Degtyareva *et al.*, *J. Phys. Condens. Matter* **17** (2005) 7955.

[2] V.F. Degtyareva, I.S. Smirnova, *Z. Kristallogr.* **222** (2007) 718–721.

10:20

Talk O-13

Title: Revisiting tungsten phosphate bronzes using the superspace formalism

Authors: •O. PÉREZ¹, L. ELCORO², J.M. PEREZ-MATO², V. PETŘÍČEK³

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Abstract: The Monophosphate Tungsten Bronzes with pentagonal tunnels $(PO_2)_4(WO_3)_{2m}$ (MPTBp) comprise a large family of compounds with $m \geq 4$ [1]. MPTBp's are conductors exhibiting properties of low dimensionality including unusual properties such as charge density, wave-driven metal-to-insulator transitions. Above the transition temperature (T_{C1}), their structure can be depicted by a regular stacking of WO_3 slabs, with a thickness proportional to m , separated by slices of phosphate PO_4 . The strong similarities with the lillianite family that exhibits modular structures recently described within the superspace formalism [2] open the route for a 4D description of MPTBp's. The unification of both the symmetry and the structure of the MPTBp's are then performed using a single superspace model ($P_{2x}W_{1-2x}O_{3-2x}$, SSG $Pnmm(00\gamma)0s0$, $\vec{q} = x\vec{c}^*$ with $x = \frac{1}{m+2}$, $0 \leq x \leq \frac{1}{2}$). X-ray single crystal diffraction data are collected above T_{C1} for different MPTBp's ($4 \leq m \leq 10$). The comparison between the refinements in both classical 3D and superspace approaches demonstrates the validity of the 4D model.

Several modulated structures are observed for the different MPTBp's below T_{C1} . The analysis of these modulations for the $m=4$ and 10 members is reported in the literature [3-5]. But the unusual distribution of the satellite reflections in the diffraction patterns reveals the potentialities of our 4D model as a tool for the determination of the modulations occurring in the MPTBp's below T_{C1} .

[1] P. Roussel, O. Pérez, Ph. Labbé, Acta Cryst. B **57** (2001) 603–632.

[2] L. Elcoro, J.M. Perez-Mato, K. Friese, V. Petříček, T. Balić-Žunić, L. Arnskov Olsenc, Acta Cryst. B **64** (2008) 684–601.

[3] P. Roussel, Ph. Labbé, H. Leligny, D. Groult, P. Foury-Leylekian, J.P. Pouget, Phys. Rev. B **62** (2000) 176–188.

[4] J. Ludecke, A. Jobst, S. van Smaalen, Europhysics Letters **49** (2000) 357–361.

[5] J. Ludecke, A. Jobst, S. Geupel, S. van Smaalen, Phys. Rev. B **64** (2001) 104105.

11:10

Invited Talk I-06

Title: Hidden degrees of freedom in composite aperiodic crystals

Authors: B. TOUDIC¹, P. GARCIA¹, L. BOURGEOIS¹, M. HUARD¹, C. ODIN¹, P. RABILLER¹, ●C. ECOLIVET¹, E. COLLET¹, P. BOURGES², G.J. MCINTYRE³, M.D. HOLLINGSWORTH⁴, T. BRECZEWSKI⁵

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Abstract: Urea-alkane inclusion compounds are characterised by two different and independent lengths: on the one hand, the helix pitch of the urea sublattice and, on the other hand, the length of the included alkane molecule defining the periodicity of the dense sublattice. All the members of this family studied so far at atmospheric pressure don't present any simple commensurate ratio for these lengths, even if, for some of them, this ratio seems rather close to commensurability. In these aperiodic structures, each sublattice modulates the other one at its own periodicity and the resulting structure can be described by the modulation functions characterised by amplitude and phase variables. Usually, in 'normal' crystals, phase variations are irrelevant but they correspond in aperiodic structures to real features which may seem to be hidden. Such a hidden aspect may also appear when describing these aperiodic structures by periodic superspaces of higher dimensionality which restore their periodicity.

We present direct observations by neutron and X-ray scattering of structural phase transitions in the urea-alkane family which are mostly driven by an intermodulation modification whereas the average structure of the sublattices don't vary concomitantly [1]. We also show that the urea-alkane family members may present a sequence of two structural phase transitions, instead of the only one quoted in literature, and that the driving force of these transitions can't be described by the coupling of a homogeneous antiferro shearing with a similar orientational guest ordering as it was presented a decade ago [2]. The aperiodicity of these compounds is clearly a relevant fact which influences profoundly the low temperatures structures and reveals a much wider unexpected variety of solutions generated by aperiodicity.

[1] B. Toudic *et al.*, Science **319** (2008) 69.

[2] R. Lynden-Bell, Mol. Phys. **79** (1993) 313.

11:50

Talk O-14

Title: Lattice dynamics in complex metallic alloys – vibrational properties of $Zn_{11}Mg_2$

Authors: •H. EUCHNER¹, M. MIHALKOVIČ², M.R. JOHNSON³, H. SCHÖBER³, A.P. TSAI⁴, S. OHASHI⁴, S. LIDIN⁵, M. DE BOISSIEU⁶

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Abstract: We report on the vibrational properties of the complex metallic alloy $Zn_{11}Mg_2$. This phase contains 39 atoms in the unit cell and is a cubic packing of 'mini Bergman' clusters linked by Zn octahedra. Thus it presents an intermediate structural complexity in between the simple Laves phases Zn_2Mg and the complex 1/1 approximant and quasicrystal $Zn(Mg)Sc$ for which experimental details and simulations of the lattice dynamics have been obtained [1,2].

Ab initio simulations, conducted with the programme package VASP, PHONON, as well as recent inelastic neutron scattering experiments have shown exceptional vibrational properties in the low energy range of the generalized vibrational density of states (GVDOS) of $Zn_{11}Mg_2$. For energies as low as a few meV a significant departure from Debye's law is evidenced in experiment and simulation, which is to our knowledge a unique feature for a close-packed metallic alloy. These low energy modes are closely linked to structural complexity and local environments of certain atoms in this 'mini Bergman' type phase. We present a detailed analysis of the eigenvectors of those low energy modes which are related to rather localized atomic motions.

[1] P. Brommer *et al.*, Vibrational properties of $MgZn_2$, *Z. Kristallogr.* **224** (2009) 97–100.

[2] M. de Boissieu *et al.*, Lattice dynamics of the Zn-Mg-Sc icosahedral quasicrystal and its Zn-Sc periodic 1/1 approximant, *Nature Materials* **6** (2007) 977–984.

12:10

Talk O-15

Title: Simple model of Mg_2Al_3 : β and β' phases**Authors:** •J. WOLNY, M. DUDA, B. KOZAKOWSKI**Address:** Faculty of Physics and Computer Science, AGH University of Science and Technology, Krakow, Poland**Abstract:** The Samson phase is one of the most complex intermetallic structures. The first description of the β - Mg_2Al_3 structure was provided by Samson [1]. Because of its complexity and potential new technical applications, during the last few years the Samson structure aroused considerable interest among crystallographers [2].Its cubic elementary cell (Fd-3m, no. 227 space group) contains 1168 atoms which are distributed over 1832 atomic positions. The lattice constant of the Samson structure is gigantic: $a = 2.8242(1)$ nm. At a temperature of 214°C , the structure undergoes a phase transformation to the rhombohedral β' - Mg_2Al_3 (space group R3m, no. 160, which is a subgroup of the Fd-3m group - index 4) with $a = 1.9968(1)$ nm, $c = 4.89114(8)$ nm. It should be pointed out that the constant c of a rhombohedral structure is practically equal to the length of the diagonal of the cubic structure. The near equivalence in length between the c of the rhombohedral β' - Mg_2Al_3 structure and the diagonal of the cubic β - Mg_2Al_3 is a consequence of lattice transformation connecting the hR cell of the β' -phase to the F cell of the β -phase.Relative distances between skeleton Al atoms belonging to different domains can be described by means of shift vectors of the length about $1/7 a_0$, where a_0 is the period length along the hexagonal planes. The shift measured along a direction perpendicular to hexagonal layers is equal to $22/3 c$ rlu and it divides the structure into equivalent domains [4].[1] S. Samson, The Crystal Structure of the phase β - Mg_2Al_3 . *Acta Crystallogr.* **19** (1965) 401–413.[2] M. Feuerbacher *et al.*, The Samson phase, β - Mg_2Al_3 revisited, *Z. Kristallogr.* **222** (2007) 259–288.[3] J. Wolny, B. Kozakowski, M. Duda, J. Kusz, Stacking of hexagonal layers in the structure of β - Mg_2Al_3 , *Phil. Mag. Lett.* **88** (2008) 501–507.

12:30

Talk O-16

Title: Low-temperature phase transition of a Zn_6Sc 1/1 cubic approximant**Authors:** •T. YAMADA¹, R. TAMURA¹, H. EUCHNER², M. DE BOISSIEU³**Addresses:** ¹Dept. of Materials Science and Technology, Tokyo University of Science, Noda, Japan ²Institute for Theoretical and Applied Physics, University of Stuttgart, Stuttgart, Germany ³SIMAP, CNRS Universite de Grenoble, Grenoble, France**Abstract:** Zn_6Sc 1/1 cubic approximant has a bcc lattice composed of a Tsai-type cluster with an orientationally disordered Zn tetrahedron at the center [1]. For Zn_6Sc , electron diffraction patterns revealed superlattice reflections at about 80K, which has been attributed to orientational ordering of the Zn tetrahedron [2]. In this study, in order to obtain insight into the detailed transition mechanism of Zn_6Sc , a single-grained crystal was prepared and investigated by X-ray diffraction. As a result, diffuse scatterings were observed at the positions of the superlattice reflections above 157K and were found to develop into Bragg peaks below T_c accompanying with lattice distortion at T_c . Due to the abrupt introduction of the lattice distortion, the transition mechanism of Zn_6Sc is found to be rather complicated compared with conventional order-disorder transitions such as β -Brass. The temperature evolution of both diffuse scatterings and superlattice reflections will be discussed in detail.[1] Q. Lin, J.D. Corbett, *Inorg. Chem.* **43** (2004) 1912.[2] R. Tamura *et al.*, *Phys. Rev. B* **71** (2005) 092203.

14:00

Invited Talk I-07

Title: Surprises in aperiodic diffraction**Authors:** M. BAAKE**Address:** Fakultät für Mathematik, Universität Bielefeld, Box, 10 01 31, 33501 Bielefeld, Germany**Abstract:** Mathematical diffraction theory is concerned with the determination of the diffraction image of a given structure and the corresponding inverse problem of structure determination. In recent years, the understanding of systems with continuous and mixed spectra has improved considerably. Moreover, the phenomenon of homometry shows various unexpected new facets. This talk reviews some of the recent results in an exemplary fashion, with some focus on joint work with U. Grimm and R.V. Moody.

14:40

Talk O-17

Title: Order and disorder in ternary decagonal tilings**Author:** N. FUJITA**Address:** Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan**Abstract:** Generalized point processes [1] have proved to be a handy tool for composing inflation rules (IRs) of quasiperiodic tilings in a controllable way. The use of the method is demonstrated by generating an interesting family of ternary quasiperiodic tilings in the plane hosted by the decagonal Bravais module. The three prototiles are the 36° rhombus, the regular pentagon, and the barrel shaped hexagon, while their number ratios are invariably $1:2:1/\tau$, respectively, with τ being the golden mean. The atomic surfaces of the ternary tilings are shown to have fractal boundaries, which are determined unambiguously by the dual maps associated with the relevant IRs. The family contains an infinite number of local indistinguishability (LI) classes which can be grouped into sub-families with distinct global symmetries (e.g., C_{10} , D_5 , etc.) as well as distinct statistics for the local arrangements of tiles. The member tilings are mutually connected through collective phason flips of the Edagawa type[2]. Phason fluctuations can be introduced into the perfect structures by exciting phason flips in a canonical Monte Carlo simulation. It is shown that different types of order and disorder can be observed depending on the energy parameters associated with specific local arrangements of tiles.[1] N. Fujita, *Acta Cryst. A* **65** (2009) 342.[2] K. Edagawa, K. Suzuki, S. Takeuchi, *Phys. Rev. Lett.* **85** (2000) 1674.

15:00

Talk O-18

Title: The hydrodynamic structure factor of quasicrystals**Authors:** •A. CHATZOPOULOS, H.-R. TREBIN**Address:** Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany**Abstract:** On the basis of the hydrodynamic equations for icosahedral quasicrystals [1] we introduce the terms of dynamic correlation and response and derive the hydrodynamic structure factor. We compute the anisotropic phasonic diffuse shoulders and illustrate the dependence on frequency. The effect of kinetic coefficients as well as of the phonon-phason coupling terms is discussed.

The results are also presented in the time domain. The connection to speckle pattern [2] is established. Anisotropic diffusion is demonstrated for several types of phason walls.

[1] T.C. Lubensky *et al.*, *Physical Review B* **32** (1985) 7444–7452.[2] S. Francoual *et al.*, *Philosophical Magazine* **86** (2005) 1029–1035.

15:20**Talk O-19**

Title: Theory of short-range order magnetic diffuse scattering in quasicrystals and application to random phason flips in the Penrose pattern

Authors: A. YAMAMOTO

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Abstract: It is well known that many alloys show diffuse scattering (DS) due to an atom arrangement with short-range order (SRO). The same holds in quasicrystals since the most quasicrystals are an alloy. The analytical formula giving the SRODS intensity of quasicrystals for x-ray has been given recently [1], while that for neutron magnetic scattering has not been derived yet. This paper will provide such a formula for the first time. As an example, this is applied to the random spin distributions in the Penrose pattern. Similarly to x-ray SRODS, the magnetic DS intensity can be calculated based on higher-dimensional models of quasicrystals. The frequency of spin pairs, which contribute to the DS intensities, is calculated from the overlapped area of the occupation domains (ODs). Except for this fact, the theory does not use the higher-dimensional description of quasicrystals. The resulting formula is quite similar to that of x-ray DS except that the former depends strongly on the spin direction. The DS intensities for two models with spins parallel and normal to the 10-fold axis will be compared with the numerical results of the same models.

[1] A. Yamamoto, Z. Krist. **223** (2008) 855–858.

11.4 Wednesday 16 September

09:00

Invited Talk I-08

Title: Modulated structures of mixed ionic conductors $A_4B_6O_{12+2\alpha}$ ($A = \text{Sr, Ba, B} = \text{Fe, In, Mg}$)

Author: A.M. ABAKUMOV

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Abstract: Anion non-stoichiometry and ordering of oxygen atoms and vacancies is one of the most intriguing problems of the crystal chemistry of oxide materials. Knowing the exact anion/vacancy ordering pattern is the crucial point to establish the link between the structure and the properties of such materials as oxide ionic conductors. Because single crystals of many oxide materials are not easily available, powder diffraction data are used for structure analysis, but if the ordering of oxygen atoms and vacancies has an incommensurate character, the structure solution becomes not a trivial matter. Using the example of the mixed ionic conductors $A_4B_6O_{12+2\alpha}$ ($A = \text{Sr, Ba, B} = \text{Fe, In, Mg}$) it will be demonstrated that a combination of electron diffraction, high resolution electron microscopy, X-ray powder diffraction and superspace structure modeling is a powerful tool for solution of such modulated structures [1-3]. These intergrowth structures consist of perovskite and rock-salt blocks, where the tetrahedral voids can be occupied by extra oxygen atoms. Alternating of the filled and empty voids gives rise to occupational and associated displacement modulations. Correlations will be made between the oxygen content, structural parameters, chemical properties (reduction/oxidation conditions) and electric transport properties of the $A_4B_6O_{12+2\alpha}$ materials and closely related $A_2B_2O_5$ brownmillerite-type compounds.

[1] M.D. Rossell *et al.*, Chem. Mater. **16** (2004) 2578.

[2] M.D. Rossell *et al.*, Chem. Mater. **17** (2005) 4717.

[3] A.M. Abakumov *et al.*, Chem. Mater. **20** (2008) 4457.

09:40

Talk O-20

Title: A general origin-independent space-group identifier applicable to space groups in arbitrary dimensions

Authors: •L. PALATINUS, G. CHAPUIS

Address: Laboratoire de Cristallographie, Le Cubotron, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Abstract: The three-dimensional space groups (SG) are nowadays usually represented by the Herman-Mauguin (HM) symbols, or the Hall symbols. However, the HM symbols cannot be obtained algorithmically from a matrix representation, and they are only defined as an entry in the International Tables for Crystallography. On the other hand, the Hall symbols can be derived from the SG's matrix representation algorithmically, and they contain implicitly the position of the origin. However, both notations require some convention-defining tables, both are limited only to standard SG settings or their trivial variations, and neither of the systems addresses the problem of algorithmic definition of a standard origin. Finally, none of these notations is generalizable to more than three dimensions, except for the extension of the HM symbols to superspace groups.

To address these problems, we have developed a new SG identifier. The proposed identifier can be algorithmically derived from the matrix representation of the SG and *vice versa*, it is origin independent, it can be derived for any SG setting, it is applicable to SGs of any dimensions, and it can be easily interpreted by a computer program. Moreover, the identifier remains concise, requiring at most 20 characters for any 3D SG in standard setting. The identifier is an ideal basis of SG handling routines in crystallographic programs, especially in cases where groups with a non-standard origin or in a non-standard setting are compared and handled.

10:00

Invited Talk I-09

Title: Advances in solution of modulated structures reflected by Jana system

Authors: •M. DUŠEK, V. PETŘÍČEK, L. PALATINUS

Address: Institute of Physics of the ASCR, v.v.i., Na Slovance 2, 18221 Prague, Czech Republic

Abstract: Number of known modulated structures is growing rapidly due to modern diffractometers and sensitive area detectors. Overlooking satellite reflections is now almost impossible and crystallographers not specialized in the field attempt to solve modulated structures. Great help for routine solution represents the generalization of the charge flipping method [1,2] for the superspace. With help of charge flipping the basic features of modulation functions can be identified in the early stage of the solution and the superspace symmetry can be easily verified. It appears that many modulated structures contain discontinuous modulation functions, crenel and sawtooth in terms of Jana software [3]. Crenel functions can be easily combined with modulation functions newly described with Legendre polynomials. They do not require special orthogonalization procedures complicating so far usage of discontinuous functions.

Finally there are news in the field of magnetic structures. The magnetic satellites can be described with superspace formalism using magnetic superspace symmetry. The obvious advantage of joint refinement against powder neutron data containing the magnetic information and single-crystal synchrotron data containing precise information about the nuclear structure has initialized large development in the field of refinement with multiple data sets.

[1] G. Ozslanyi, A. Suto, *Acta Cryst. A* **60** (2004) 134–141.

[2] L. Palatinus, G. Chapuis (2007), *J. Appl. Cryst.* **40** (2007) 786–790.

[3] <http://www-xray.fzu.cz/jana>

11:10

Invited Talk I-10

Title: Terminations, adsorption sites, and metal nano island nucleation and growth on i-Al-Pd-Mn quasicrystal surfaces

Authors: •B. ÜNAL, P.A. THIEL

Address: Ames Laboratory and Departments of Materials Science and Engineering, of Chemistry, Iowa State University, Ames, IA 50011

Abstract: We have analyzed bulk structure models for icosahedral Al-Pd-Mn in terms of the densities, compositions, and interplanar spacings for the fivefold planes. Each of the deterministic models that we have investigated contains paired planes – layers that can be separated into two main families on the basis of three features: the gap separating the layer from the nearest atomic plane, the relative densities of the two planes, and the Pd content in the topmost plane. Based on the experimental data and other arguments, we have concluded that the family with no Pd in the top plane is the favored one. We have also examined the nature of the local motifs – dark stars and white flowers – seen in scanning tunneling microscopy (STM) images. We have found that these features are heterogeneous in terms of their chemical decoration, even within a single model. Both sites are also structurally heterogeneous in the bulk models, and the structural variation is consistent with STM measurements. We have found that there are correlations between the density of these features and the step heights.

Using STM, we have investigated the nucleation and growth of Ag islands on the fivefold surface of an icosahedral Al-Pd-Mn quasicrystal. Our analysis of the data revealed that the island density does not vary between 127K and 300K while it scales with temperature above 300K, which indicates that nucleation is heterogeneous. We have developed a rate equation model to understand this behavior. Our model suggests that the smallest stable cluster is formed by 6 Ag atoms. Together with the potential energy surface, the model also suggests that the nucleation happens at dark star sites, because they are stronger adsorption sites for Ag adatoms. In addition to the nucleation, we have investigated the growth of the Ag islands on the same surface. We have observed that at 365K, Ag quickly segregates into 3-layer-high, mesa-like nano islands. Our step dynamics modeling indicates that the transition from 2-D to 3-D growth is triggered by strain buildup for larger islands and enhanced binding in higher layers. However, the height selection is controlled by quantum size effects.

11:50

Talk O-21

Title: Quantum size effects in the thin metal films grown on complex metallic alloy surfaces

Authors: •A.K. SHUKLA¹, J. LEDIEU¹, E. GAUDRY¹, B. ÜNAL², C.J. JENKS², A.R. ROSS², T.A. LOGRASSO², P.A. THIEL², J.-M. DUBOIS¹, V. FOURNÉE¹

Addresses: ¹Institut Jean Lamour, Département Chimie et Physique des Solides et des Surfaces, UMR 7198 CNRS-Nancy-Université-UPVM, Ecole des Mines, Parc de Saurupt, 54042 Nancy, France ²Ames Laboratory, Department of Chemistry, Iowa State University, Ames, Iowa 50011, USA

Abstract: Quantum size effects (QSE) in thin metal films have attracted immense interest in the last few decades. They arise from electron confinement within nanostructures, normally induced by a gap in the substrate electronic structure. Recently, magic height islands has been reported in several metal/quasicrystal systems by scanning tunnelling microscopy (STM) and quantum well states have been observed by photoemission spectroscopy (UPS), suggesting that electron confinement is a rather general effect on quasicrystalline substrate. Here we will report on two new systems for which QSE are observed, namely Ag and Bi films grown on either the 5-fold surface of icosahedral (i)-Al-Cu-Fe quasicrystal and the (100) surface of the Al₁₃Co₄ periodic approximant respectively. This will allow us to discuss the possible origins of the electron confinement based on scanning tunnelling microscopy and photoemission spectroscopy data.

12:10

Talk O-22

Title: About the chemistry of the termination 5f planes in surface studies of *i*-AlPdMn

Authors: M. QUIQUANDON¹, B. ÜNAL², P.A. THIEL², •D. GRATIAS¹

Addresses: ¹Laboratoire d'Etude des Microstructures, CNRS-ONERA, Châtillon, France ²AMES Laboratory, IOWA State University, Ames, USA

Abstract: It will be proposed, in the example of the *i*-AlPdMn phase, some theoretical arguments demonstrating that the observed rich Al surfaces may can correspond to actual bulk properties and structural models proposed to this phase with no need of a possible Al segregation on the surface. Indeed, the most recent surface studies of the 5-fold termination planes in *i*-AlPdMn [1] show that termination planes are made of two close planes containing essentially Al at the upper one and Al and Pd at the second one.

Perfect unrelaxed chemical models close to the description proposed in [2] are compared to experimental diffraction data [3]. Even though the comparison shows that the chemical decoration has a rather limited influence on the global R-factor, there is a clear tendency in favoring models having pure Al on the atomic surface placed on the node *n* in the perpendicular space. Such a result means that the termination plane is composed only with Al that is in good agreement with the surface studies.

[1] B. Unal, C.J. Jenks, P.A. Thiel, Phys. Rev. B **77** (2008) 195419.

[2] M. Quiquandon, D. Gratias, Phys. Rev. B **74** (2006) 214205.

[3] M. Boudard *et al.*, J. Phys. Condens. Matter **4** (1992) 10149.

12:30

Talk O-23

Title: STM Studies of high symmetry surfaces of i-In-Ag-Yb quasicrystals

Authors: •M. SHIMODA¹, C. CUI², S. OHASHI², H.R. SHARMA³, P.J. NUGENT³, H. TAKAKURA⁴, A.P. TSAI²

Addresses: ¹National Institute for Materials Science, Photocatalytic Materials Center, Tsukuba, 305-0047, Japan ²Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, 980-8577, Japan ³Surface Science Research Centre and Department of Physics, The University of Liverpool, Liverpool L69 3BX, UK ⁴Division of Applied Physics, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, Japan

Abstract: We present STM studies on the high symmetry surfaces of i-In-Ag-Yb quasicrystal. Step-terrace features and in-plane atomic arrangements of the 2-, 3- and 5-fold surfaces are analyzed using the refined structure model [1]. For the 5-fold surface, it is found that both the step height distribution and the atomic arrangement are successfully explained by bulk termination at Yb-rich planes which intersect the cluster centers. Our preliminary study suggests that this is also true for the 2-fold surface. Interestingly, these planes associated with the 2-fold surface have the maximum atomic density. However, this is not the case for those with the 5-fold surface.

[1] H. Takakura *et al.*, Nature Materials **6** (2006) 58.

11.5 Thursday 17 September

09:00

Invited Talk I-11

Title: Geometrical constraints for the formation of 7-fold axial symmetries

Authors: •C. BECHINGER^{1,2}, J. MIKHAEL², M. SCHMIEDEBERG³, H. STARK³, J. ROTH^{1,4}

Addresses: ¹2. Physics Institute, University of Stuttgart, 70569 Stuttgart, Germany ²Max-Planck-Institute for Metal Research, Stuttgart, Germany ³Institute for Theoretical Physics, TU-Berlin, 10623 Berlin, Germany ⁴Institute for Theoretical and Applied Physics, University of Stuttgart, 70569 Stuttgart, Germany

Abstract: Although by now almost 100 different quasicrystals have been identified, not a single one has 7-fold symmetry. The reason for this is not clear in particular, since tilings with any n-fold axial symmetry (n being an arbitrary integer number) are easily obtained. Here we report on the role of geometrical constraints which may obstruct the formation of certain rotational symmetries. In our experiments, we create 5- and 7-fold quasiperiodic standing laser fields which interact due to optical forces with a monolayer of negatively charged microparticles. In contrast to 5-fold light patterns which are easily transferred to the particle monolayer, even at strong laser intensities this is not true for the 7-fold laser fields. In the latter case we observe large periodic domains which are found to be always terminated at positions where the underlying quasicrystalline light pattern exhibits highly symmetric motives. When calculating the mean distance of such motives for different rotational symmetries, we find that it differs by more than two orders of magnitude between observed and not observed quasicrystalline symmetries. Based on this observation we suggest a simple geometrical model which can explain why proliferation of certain rotational symmetries is unfavorable.

09:40

Talk O-24

Title: Colloidal particles on substrates with decagonal symmetry

Authors: •M. SCHMIEDEBERG¹, J. MIKHAEL², J. ROTH³, C. BECHINGER^{2,4}, H. STARK¹

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Abstract: Colloidal particles are an attractive model system for studying features of atomic systems. In recent years, there has been a lot of interest in growing quasicrystalline films by depositing atoms on the surfaces of quasicrystals. We aim to contribute to these investigations by concentrating on the structural features of the substrate potential leaving aside chemical details. We study a 2D charge-stabilized colloidal suspension in quasicrystalline potentials with decagonal symmetry that in experiments is realized by five interfering laser beams.

We discover a rich phase behavior which we illustrate by phase diagrams as a function of particle density and strength of the substrate potential. Especially, at medium substrate strengths, when the colloidal ordering results from a competition of the colloidal interaction and the substrate potential, interesting intermediate phases occur. For example, in dilute systems, we observe a quasicrystalline phase which exhibits bond orientations in 20 different directions [1]. On the other hand, for larger densities, the system locks into a highly ordered phase that is close to an Archimedean tiling [2].

[1] M. Schmiedeberg, H. Stark, Phys. Rev. Lett. **101** (2008) 218302.

[2] J. Mikhael, J. Roth, L. Helden, C. Bechinger, Nature **454** (2008) 501.

10:00

Talk O-25

Title: Spontaneous formation of a dense aperiodic crystal from hard tetrahedra

Authors: •M. ENGEL¹, A. HAJI-AKBARI¹, A.S. KEYS¹, S.C. GLOTZER^{1,2}

Address: ¹Department of Chemical Engineering, University of Michigan, Ann Arbor MI 48109, USA ²Department of Materials Science and Engineering, University of Michigan, Ann Arbor MI 48109, USA

Abstract: The best packing of hard tetrahedra remains an unsolved problem, and there has been much recent debate. We simulate a system of mathematically smooth, hard regular tetrahedra using NPT Monte Carlo simulations and determine the density-pressure equation of state. We find disordered and aperiodic packings with densities that significantly exceed the close-packed hard sphere FCC packing density of 0.7405. Our findings thus demonstrate that tetrahedra obey a conjecture by Ulam that spheres pack with a lower maximum packing density than any other hard convex object, despite recent speculation to the contrary. We show that the system is able to achieve such high packing densities by the local ordering of tetrahedra into certain favorable motifs, forming larger structures that pack efficiently in both jammed and aperiodic structures. Our results provide the first example of a non-simple crystal formed spontaneously from hard particles, and demonstrate how particle shape and entropy may be exploited to achieve highly complex structures.

10:20

Talk O-26

Title: Stability of quasicrystals composed of soft isotropic particles

Authors: K. KAN¹, H. DIAMANT², •R. LIFSHITZ¹

Address: ¹School of Physics & Astronomy, Tel Aviv University, Tel Aviv 69978, Israel ²School of Chemistry, Tel Aviv University, Tel Aviv 69978, Israel

Abstract: In recent years we have witnessed the exciting experimental discovery of soft matter with nontrivial quasiperiodic long-range order—a new form of matter called a *soft quasicrystal* [1,2]. At the last Aperiodic conference [3] we offered a conjecture, suggesting that the existence of two natural length-scales, along with three-body interactions, may constitute the underlying source of their stability. By using a coarse-grained description for a system of soft isotropic particles—to model the experiments of Zeng *et al.* [1]—we show here that indeed this is the case. Whereas we find that a variety of isotropic pair-potentials are capable of setting the two required length scales, it is the entropy that is responsible for introducing effective three-body interactions in these systems. This unique interplay between the roles of energy and entropy in stabilizing soft quasicrystals may shed new light on the more evasive question of the stability of solid-state quasicrystals.

[1] Zeng *et al.*, *Nature* **428** (2004) 157.

[2] Hayashida *et al.*, *Phys. Rev. Lett.* **68** (2007) 195502.

[3] Lifshitz & Diamant, *Phil. Mag.* **87** (2007) 3021.

11:10

Invited Talk I-12

Title: Recent developments in the mathematics of grain boundaries

Authors: •M. LOQUIAS^{1,2}, P. ZEINER¹

Addresses: ¹Faculty of Mathematics, University of Bielefeld, Germany ²Institute of Mathematics, University of the Philippines Diliman, Quezon City, Philippines

Abstract: For several decades, coincidence site lattices or CSLs have been used to study and classify the structure of grain boundaries in crystals. Given a lattice Γ in \mathbb{R}^d and $R \in O(d)$, a coincidence site lattice is formed when $\Gamma \cap R\Gamma$ is a sublattice of finite index in Γ . These coincidence isometries form a group, denoted $OC(\Gamma)$.

After the discovery of quasicrystals, there was a renewed interest in CSLs because quasicrystals also have grain boundaries. This led to the examination of CSLs from a more mathematical point of view so that results for lattices may be readily extended to aperiodic situations, which is possible via their underlying translation modules, in particular, modules with 5, 8, 10, and 12-fold symmetry.

In this talk, we will look at some of the recent progress made on the theory of CSLs as well as CSMs (coincidence site modules). We will start with results on the group of coincidence isometries $OC(\Gamma)$ and its relationship with the group of similarity rotations. We then discuss how to extend the notion of a colour symmetry, originally defined for symmetries of a lattice, to coincidence isometries of the lattice and its consequences. Finally, we address the coincidence problem for shifted lattices which is equivalent to the problem of affine coincidences of a lattice.

11:50

Talk O-27

Title: Colour groups in tilings with singularities

Author: R. LÜCK

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Abstract: Colour symmetries have been discussed for euclidian periodic and quasiperiodic [1,2] as well as for hyperbolic tilings [3]. The advantage of this research is – beside the aesthetics of the results – a deeper understanding of superstructures due to chemical ordering and of coincidence site lattices. The presentation will be focussed on regular tilings with singularities which were described by Grünbaum and Shephard [4]. Such tilings are selfsimilar with a scaling factor like in quasiperiodic patterns. Moreover, periodic arrangements of singularities will be introduced for the visualisation of special hyperbolic tilings. The number of possible colourings in the considered tilings are not only determined by the symmetry of the tiling as described in [1] and [3] but additionally by the rotational symmetry of the singularities. The number of possible colourings was found to be limited or at least reduced. Examples including phyllotactic analysis will be presented and discussed.

[1] M. Baake, J. Phys. A 30 (1997) 2687.

[2] R. Lück, Phil. Mag. 88 (2008) 2049.

[3] D. Frettlöh, Z. Krist. 223 (2008) 773.

[4] B. Grünbaum, C.G. Shephard, Tilings and Patterns, Freeman, New York (1987).

12:10

Talk O-28

Title: In search of magnetic long-range order on quasiperiodic tilings

Author: E.Y. VEDMEDENKO

Address: Institute for Applied Physics, University of Hamburg, Germany

Abstract: We use Monte Carlo calculations to analyze magnetic ordering on the Penrose and Amman-Beenker tilings, relevant for two-dimensional molecular adsorbates on quasicrystalline surfaces and for nanomagnetic arrays. Ground states corresponding to the short-range exchange interactions [1] will be compared with those corresponding to the long-range multipolar coupling [2]. Our initial investigations are restricted to multipolar rotors of rank one through four positioned on the vertices of the corresponding tiling. At first sight, the ground states of odd-parity multipoles on the rhombic Penrose tiling seem to exhibit long-range order, in agreement with previous investigations of dipolar systems. Yet, careful analysis performed here establishes that long-range order is absent for all types of rotors, and only short-range order on the Penrose tiling exists. Nevertheless, we show here that short-range order suffices to yield a superstructure in the form of the decagonal Hexagon-Boat-Star tiling.

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

[2] E.Y. Vedmedenko, S. Even-Dar Mandel, R. Lifshitz, Phil. Mag. **88** (2008) 2197.

12:30

Talk O-29

Title: Aperiodic sequences of quantum dots in external magnetic and electric fields

Authors: •N.E. KAPUTKINA¹, YU.E. LOZOVIK², R.F. MUNTYANU¹, YU.KH. VEKILOV¹

Addresses: ¹State Technological University "Moscow Institute of Steel and Alloys", Moscow, Russia ²Institute of Spectroscopy, Academy of Sciences of Russia, Troitsk, Russia

Abstract: In the present work we investigated electronic and excitonic excitations in aperiodic sequences of quantum dots (QDs). We studied such systems analytically and numerically taking into account inter-dot interaction and influences of magnetic and electric fields. We investigated single-particle and two-particle energy spectrum of chains of QDs with Fibonacci, Tue-Morse, Rudin-Shapiro, Cantor, and double-period sequences.

Energy spectrum of a single QD and sequences of QD was determined using perturbation theory. QD pair interaction (nearest neighbor interaction) was taken into consideration and critical values for α (steepness of confining potential) and d (distance between neighboring QD) were obtained so one could switch from a separate QD chain to pairs of neighboring QD sequence. Single-particle and two-particle tunneling probability was taken into consideration: transmission coefficient was determined using quasi-classical approximation and range of values of α , d when tunneling is essential was estimated.

An external electrical and magnetic field effect on electron localization was taken into consideration, an effective steepness of confining potential in magnetic field was appeared as new control parameter of a problem. External magnetic field influences also on the wave functions overlapping and tunneling probability. Energy spectrum of an aperiodic QD sequences in external magnetic field was obtained. Possibility to tune the state of the system by magnetic field was studied. The increase of the external electrical field shifts the energy states of the particle in a QD and contributes to particle localization. The localization of the excitations is possible at the finite values of the perturbation in the case of aperiodic sequences of QDs (contrary to the case of periodical sequences).

14:00

Talk O-30

Title: Atomic short-range and medium-range order in Al-Ni-Co decagonal quasicrystals

Author: H. ABE

Address: Dept. of Materials Science and Engineering, National Defense Academy, Yokosuka 239-8686, Japan

Abstract: Diffuse scattering from atomic short-range order (SRO) and medium-range order (MRO) [1] are analyzed by Monte Carlo simulations. The diffuse scattering is relating to an order-disorder phase transition [2] on $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, which is regarded as one of perfect quasicrystals. Moreover, three kinds of atomic pairs (Al-Ni, Ni-Co and Co-Al) are decomposed by quantitative measurements and analysis. By a combination of SRO and MRO effects, the calculated diffuse scattering is in good agreement with the experimental one.

[1] H. Abe, J. Phys. Soc. Jpn. **76** (2007) 094601.

[2] H. Abe, H. Saitoh, T. Ueno, H. Nakao, Y. Matsuo, K. Ohshima, H. Matsumoto, J. Phys.: Condens. Matter **15** (2003) 1665.

14:20

Talk O-31

Title: Modeling of decagonal quasicrystals

Authors: •S. DELOUDI, W. STEURER

Address: Laboratory of Crystallography, ETH Zurich, Switzerland

Abstract: Among the axial quasicrystal structures, the system Al-Co-Ni is the best studied, but the discussion about the structures within this system is still ongoing. Its suitability as a model system is excellent because of several reasons. The phase diagram is well investigated and shows a wide range of modifications of the decagonal phase as a function of composition and temperature. Large single crystals can be easily grown, and electron-microscopic and surface-imaging methods can be used due to the short translation period along the tenfold axis. In a previous work [1] we have presented a fundamental cluster with 20 Å diameter which makes it possible to model all decagonal phases in the system Al-Co-Ni (including the approximants) systematically, with small changes in the atomic structure. We have now extended the modeling to the systems Al-Co-Cu and Al-Fe-Ni, showing that it is possible to derive all these complex phases from only one building principle. Furthermore, it is even possible with this approach to predict and explain atomic flip positions within the structures of all phases. Here, we will concentrate on the geometrical aspects of the models for Al-based decagonal QCs with a four-layer periodicity, such as the generation of flip positions and superstructures, and we will discuss the agreement of our models with experiment.

[1] S. Deloudi, W. Steurer, Philos. Mag. **87** (2007) 2727.

14:40

Talk O-32

Title: Spectroscopic study on chemical ordering of transition metals in decagonal Al-Co-Ni and Al-Co-Cu quasicrystals

Authors: •M. INUKAI^{1,2}, K. SODA¹, M. KATO¹, S. YAGI¹, Y. TEZUKA³, Y. YOKOYAMA⁴, T. MURO⁵

Addresses: ¹Graduate School of Engineering, Nagoya University, Nagoya, Japan ²Venture Business Laboratory, Nagoya University, Nagoya, Japan ³Faculty of Science and Technology, Hirosaki University, Hirosaki, Japan ⁴Institute of Materials Research, Tohoku University, Sendai, Japan ⁵Japan Synchrotron Radiation Research Institute, Sayo, Japan

Abstract: The preferred occupation at the transition metal (TM) sites in the decagonal unit cluster [1] of two-dimensional Al-Co-Ni and Al-Co-Cu quasicrystals has been investigated by comparing their experimental electronic structures with those of the unit clusters calculated by a discrete variational $X\alpha$ methods. Analysis on the bonding character and bond energy for local clusters around the TM sites shows that Al-Co-Cu favors the Cu and Co occupations at the first and second inner TM sites, respectively, and hence the chemical order of these TM's, while the small energy difference in the Ni and Co occupations at those TM sites suggests the large chemical disorder of the transition metals in Al-Co-Ni.

[1] K. Hiraga, Adv. Imaging and Electron Phys. **122** (2002) 1.

15:00

Talk O-33

Title: Structure of B-Ti-Ru decagonal approximant crystals

Authors: •Y. MIYAZAKI¹, J.T. OKADA², E. ABE³, Y. YOKOYAMA⁴, K. KIMURA¹

Addresses: ¹Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Japan ²Japan Aerospace Exploration Agency, Tsukuba, Japan ³Department of Materials Science and Engineering, The University of Tokyo, Tokyo, Japan ⁴Institute for Materials Research, Tohoku University, Sendai, Japan

Abstract: We have reported aperiodic tiling structure possessing apparent decagonal symmetry in melt-quenched B-Ti-Ru alloys at QC07, IUCr08 and ISBB08. Its HAADF-STEM images correspond to the decagonal quasicrystal (DQC) theoretically predicted in B-Mg-Ru system by Mihalkovic and Widom [1], though the samples contain inhomogeneity and quite many disorders. We have also observed variety of approximant crystals of the DQC in the same alloys. High-quality boron-based DQC has not yet been obtained, but studying these approximant crystals may be meaningful to understand the structures, stability and physical properties of boron-based quasicrystals.

In the melt-quenched alloys, forming approximant crystals are; tessellation of two differently oriented hexagon subunits similar to $B_4Mg_2Ru_5(\alpha)$ and $B_4Sc_2Ru_5$ [2] as reported by Rosenberg and Steurer; and several tessellations consisting of hexagon and boat with long modulated periodicities, which correspond to $\beta, \delta, \epsilon \dots$ in B-Mg-Ru system [3,4] whose lattice parameters a equals 2.2, 3.5, 8.4 ... nm, respectively. Results of long time annealing (1373K–1673K, 72–144h) indicate that α and at least one of the long-period structures are stable phase. We will show the detail of HAADF-STEM images and results of analysis of powder X-ray diffraction on the presentation.

[1] M. Mihalkovic, M. Widom, Phys. Rev. Lett. **93** (2004) 095507.

[2] P. Rogl, J. Solid State Chem. **55** (1984) 262.

[3] Y. Miyazaki, J.T. Okada, K. Kimura, Philos. Mag. **87** (2007) 2701.

[4] Y. Miyazaki, J.T. Okada, E. Abe, K. Kimura, Philos. Mag. **88** (2008) 1935.

15:20

Talk O-34

Title: Solution of the average structure of basic Co-rich decagonal Al-Ni-Co based on a five-dimensional model

Authors: •A. STRUTZ¹, A. YAMAMOTO², W. STEURER¹

Addresses: ¹Laboratory of Crystallography, Departement of Materials, ETH Zurich, 8093 Zurich, Switzerland ²National Institute for Materials Science, Namiki 1, Tsukuba, Ibaraki, 305-0044, Japan

Abstract: An average structure solution of the decagonal basic Co Al_{72.5}Co_{18.5}Ni₉ quasicrystal was determined based on the refinement of single-crystal five-dimensional data using a higher dimensional structure model. The determined higher dimensional space group is non-centrosymmetric $P\bar{1}0m2$. The best-fit model structure with 229 parameters resulted in $wR = 0.109$ and $R = 0.1263$ for 957 reflections. The model is consistent with the closely related W-phase approximant.

16:15

Science in Fiction

Title: "Quasi-fictional"

Author: Ann Lingard

Abstract: Why is one of the characters in Ann Lingard's latest novel, *The Embalmer's Book of Recipes*, a Liverpool-based mathematician working on aperiodic order? Come and relax at an informal session during which Ann — with the help of a few short readings and lots of images — will talk about the fun and difficulties of putting (a little) science into fiction. See also www.annlingard.com.

The talk is followed by sales and signing of *The Embalmer's Book of Recipes* ('A powerful and haunting story of genetic difference, interwoven with maths, taxidermy, and the tragedy of foot and mouth disease. An exhilarating and compelling read.' Professor Sir John Sulston, Nobel Laureate; 'My favourite fictional mathematician.' Dr Tony Mann, LMS).

11.6 Friday 18 September

09:00

Invited Talk I-13

Title: Phase transitions and modulated structures of Λ -Co(sepulchrate)-trinitrate at low temperatures

Authors: •A. SCHÖNLEBER¹, S. VAN SMAALEN¹, W. MORGENROTH², F.K. LARSEN³

Addresses: ¹Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany
²Institute of Geosciences, University of Frankfurt, Frankfurt am Main, Germany. ³Department of Chemistry, University of Aarhus, Aarhus, Denmark

Abstract: Λ -Co(sepulchrate)-trinitrate, $C_{12}H_{30}N_8Co^{3+} \cdot 3(NO_3)^-$, crystallizes at room temperature in symmetry $P6_322$ [1]. Applying spectroscopic measurements, phase transitions have been observed at $T_1 = 133$ K and at $T_2 = 106$ K [2]. By single-crystal neutron diffraction upon cooling the appearance of satellite reflections in the diffraction pattern at $T_1 = 133$ K was discovered [3]. Additional phase transitions have been observed at $T_2 = 107$ K and at $T_3 = 98$ K.

We have performed single-crystal X-ray diffraction at Hasylab (DESY, Hamburg) in dependence on temperature. The main reflections are surrounded by satellites up to second order. All observed peaks can be indexed in an hexagonal unit cell with two \mathbf{q} -vectors $(\sigma, \sigma, 0)$ and $(-\sigma, 2\sigma, 0)$. We will present the results of the data analysis.

[1] Dubicki *et al.*, J. Phys. Chem. **88** (1984) 4254.

[2] Dubicki *et al.*, Chem. Phys. Lett. **74** (1980) 393.

[3] Larsen *et al.*, in: Molecular structure: Chemical reactivity and biological activity, Stezowski *et al.* (eds.), IUCr, Oxford University Press (1988).

09:40

Talk O-35

Title: Quasicrystals of higher irrationality

Author: J. ROTH

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Abstract: Up to now only n -fold symmetric quasicrystals with quadratic irrationalities, i.e. 5-, 8-, 10-, 12-fold, and icosahedral symmetry have been observed in nature. Quasicrystals with cubic (7- and 9-fold) or higher irrationalities have been studied only in static artificial nanostructures. Only recently it has become possible to explore non-static systems realized by colloids trapped in n -fold symmetric laser potentials.

These developments revived the interest in quasicrystals with higher irrationalities. We will first review what is known about such quasicrystals with respect to embedding dimensions, inflation/deflation, matching rules and stability. Cut-and-projection and substitution methods typically yield larger differences for these quasicrystals especially in their diffraction properties.

In a second step we will present new results in particular of the difference between quasiperiodic laser potentials and tilings. We evaluate the possibilities to generate binary tilings from general rhombus and triangle tilings. We count the vertex frequencies of high symmetry sites which play an important role in the structure formation of colloids. Furthermore there is a close connection between the high symmetry sites and binary tilings. We finally determine local isomorphism classes of laser potentials with respect to non-trivial phase shifts which is, like the high symmetry sites, determined by the property of the Wyckoff positions of highest order.

10:00

Talk O-36

Title: Local disorder in decagonal Al-Cu-Co quasicrystals explored by the three-dimensional pair distribution function

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Abstract: Pair Distribution Function (PDF) analysis of X-ray or neutron scattering intensities allows us to investigate structural disorder of complex materials. Common PDF analysis, however, is carried out on one-dimensional scattering intensities of powder diffraction experiments, and thus, it restricts our view to the one-dimensional rotational projection of the interatomic vector distribution. By the use of three-dimensional single crystal data, the method presented here, is an upgrade of PDF analysis to the actual orientation of interatomic vectors in three-dimensional space. In this way, information about locally disordered crystal structures becomes accessible in an easy and direct manner [1]. The application of the three-dimensional PDF (3d-PDF) analysis is demonstrated, using a decagonal $\text{Al}_{65}\text{Cu}_{20}\text{Co}_{15}$ quasicrystal. A 3d-PDF was calculated by Fourier transform of the diffuse interlayers of a single crystal X-ray dataset. This PDF shows strong pair correlations of lengths less than $\sim 14.5 \text{ \AA}$. Within this range, locally disordered structure motifs of the crystal structure could be identified. Optimisation of these motifs by the use of evolutionary computing affords a well-fitting structural model of disorder.

[1] Ph. Schaub, Th. Weber, W. Steurer, *Phil. Mag.* **87** (2007) 2781–2787.

10:20

Talk O-37

Title: The uniaxially aperiodic structure of a thin Cu film on 5-fold i-Al-Pd-Mn

Authors: •K. PUSSI¹, M. GIERER², R.D. DIEHL¹

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Abstract: The growth of Cu on the 5-fold surface of i-Al-Pd-Mn has many curious features [1, 2]. By fitting the measured parameters from both the STM and LEED experiments, it was possible to derive a basic structure model. This model consists of 5 rotated domains, having a periodicity of 2.53 \AA in one direction and the substrate Fibonacci structure in the perpendicular direction. The Fourier transform of such a model is consistent with the observed LEED patterns [2]. However, the atomistic structure within this model cannot be determined from the spot locations in the LEED patterns alone. For this, the spot intensities must be analyzed. An earlier LEED intensity analysis of this surface considered atomistic models based on fcc(100), fcc(111), fcc(110) and a stepped body-centered tetragonal (bct) surface [3]. In the study reported here, we have extended the dynamical LEED analysis to different models, including the Archimedes tiling type structures recently observed in two-dimensional colloidal suspensions [4,5], and we have revisited models based on vicinal surfaces. This LEED analysis shows that a vicinal body-centered tetragonal structure provides a better model for the observed aperiodic Cu film than various two-dimensional models. The best-fit result consists of a bct film with $a = 2.88 \text{ \AA}$, $b = 2.55 \text{ \AA}$ and $c = 2.88 \text{ \AA}$, with the surface at an angle of 13.28° relative to the a-b plane [6].

[1] J. Ledieu, J.-T. Hoeft, D.E. Reid, J. Smerdon, R.D. Diehl, T.A. Lograsso, A.R. Ross, R. McGrath, *Phys. Rev. Lett.* **92** (2004) 135507.

[2] J. Ledieu, J. T. Hoeft, D. E. Reid, J. A. Smerdon, R. D. Diehl, N. Ferralis, T. A. Lograsso, A. R. Ross, R. McGrath, *Physical Review B* **72** (2005) 035420.

[3] K. Pussi, D.E. Reid, N. Ferralis, R. McGrath, T.A. Lograsso, A.R. Ross, R.D. Diehl, *Philosophical Magazine* **88** (2008) 2103.

[4] J. Mikhael, J. Roth, L. Helden, C. Bechinger, *Nature* **454** (2008) 501.

[5] M. Schmiedeberg, H. Stark, *Phys. Rev. Lett.* **101** (2008) 218302.

[6] To be published in *Journal of Physics: Condensed Matter* (2009).

11:10

Talk O-38

Title: Evolution and structural transition of quasicrystalline phases in Al-Fe-Cu-Cr and Al-Fe-Cu-Mn alloys during high energy ball milling

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Abstract: The quasicrystalline phases have been synthesized by melting the individual elements as well as by mechanical alloying of the concerned elements using high energy ball milling. The transformation of icosahedral and decagonal quasicrystalline phase to various disordered states and to crystalline as well as amorphous phase in Al-Fe-Cu-Cr and Al-Fe-Cu-Mn alloys during milling of the pre-alloyed material and also the individual elements have been studied extensively. It is known that the mechanisms of structural transformation for quasicrystalline materials have not yet been understood. In fact, the suitable experimental condition cannot be predicted for the desired structural and microstructural transformations during milling process. Therefore, there is a need to understand the structural stability of quasicrystalline phases and their structural relations with the related complex crystalline phases. The main objective of the proposed work would be to investigate into the transformation mechanism during mechanical alloying/ milling. The mechanical milling of a quasicrystalline alloy was carried out a high-energy ball mill (Szegvari attritor) by varying milling time up to 40h under liquid hexane medium and at various milling intensity. X-ray diffraction was carried out for evaluating the lattice strain, lattice parameters and crystallite sizes of the mechanically milled samples. The evolution of nano icosahedral and nano decagonal phases as well as crystalline phases was found to occur. The subsequent thermal treatment led to the structural ordering in the concerned phases. The implication of the evolution of various phases, their structural correlations and their relative stability will be discussed.

11:30

Talk O-39

Title: Low-temperature TEM observations of Cd₆M (M=Sr, Pr, Nd and Sm) approximants

Authors: •K. NISHIMOTO, M. MURAKI, T. SATO, R. TAMURA

Address: Department Materials Science & Technology, Tokyo University of Science, Chiba 278-8510, Japan

Abstract: Most of Cd₆M (M=Ca, rare earth) approximants have a *bcc* lattice at room temperature [1] and are composed of Tsai-type clusters. At the center of the Tsai-type cluster, there is an orientationally disordered Cd tetrahedron except for Cd₆Eu and Cd₆Ce. For Cd₆Yb, an occurrence of a phase transition was discovered at 110K [2], which has been attributed to orientational ordering of the Cd tetrahedron at the center of the Tsai-type cluster. In the present study, we have investigated the low-temperature structures of Cd₆M (M=Sr, Pr, Nd and Sm) compounds by transmission electron microscopy (TEM) in order to obtain insight into the occurrence of a phase transition at a low temperature. For Cd₆Nd, superlattice reflections appear in a commensurate manner to the fundamental reflections at low temperatures, which indicates that Cd₆Nd undergoes a phase transition to a $\sqrt{2}a \times a \times \sqrt{2}a$ C-centred monoclinic lattice with space group *C2/c*. The occurrence of the phase transition is explained by orientational ordering of the tetrahedron. Results on other Cd₆M (M=Sr, Pr, Nd and Sm) approximants will be discussed in details.

[1] C.P. Gomez *et al.*, Phys. Rev. B **68** (2003) 024203.

[2] R. Tamura *et al.*, Jpn. J. Appl. Phys. **41** (2002) L524.

11:50

Talk O-40

Title: Hall effect of the Y-Al-Ni-Co and *o*-Al₁₃Co₄ decagonal approximants

Authors: •J. IVKOV¹, M. KOMELJ², A. SMONTARA¹, J. DOLINŠEK², P. GILLE³

Addresses: ¹Institute of Physics, Zagreb, Croatia ²J. Stefan Institute, University of Ljubljana, Ljubljana, Slovenia ³Department of Earth and Environmental Sciences, Ludwig-Maximilians-Universität München, München, Germany

Abstract: The Hall effect in Y-Al-Ni-Co (*m*-Al₇₆Co₂₂Ni₂) and *o*-Al₁₃Co₄ single crystals has been measured for all the combinations of the electrical current and magnetic field directions, and in the temperature interval from 90 to 370 K. In these intermetallics the Hall coefficient R_H exhibits well defined anisotropy and only a weak temperature dependence. R_H is negative electron-like or zero for the magnetic field perpendicular to the plane that corresponds to the quasiperiodic plane in decagonal quasicrystals, and is positive hole-like or zero for the magnetic field parallel to this plane. The results for the anisotropy of R_H are well correlated to the anisotropy of R_H in *d*-Al-Ni-Co-type decagonal quasicrystals. Therefore, the anisotropy in these both crystalline and quasicrystalline materials originates from the specific stacked-layer structure and the chemical decoration of the lattice. The investigated anisotropic R_H in crystalline Al-Co-Ni intermetallics was reproduced theoretically by *ab-initio* calculation using Boltzmann transport theory and the calculated anisotropic Fermi surface.

11.7 Poster presentations

Poster P-01

Title: Direct evidence of phason-perturbated Penrose-tile atomic structure through ultrahigh-resolution STEM imaging

Authors: •E. ABE¹, T. SEKI¹, S.J. PENNYCOOK²

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Abstract: Are quasicrystals energetically or entropically stabilized? This has been the long-standing key issue to understand why they form instead of competing periodic crystals. Even for the best-ordered quasicrystalline compounds, we still observe substantial diffuse scattering to originate from phason-related fluctuations. Quantitative evaluation of phason-related atomistic disorders is therefore important to understand thermodynamic stability of quasicrystals, but it is difficult to see the defect configurations in a real-space structure. Here we use state-of-the-art ultrahigh-resolution scanning transmission electron microscopy (STEM) to identify the atomic occupations at individual sites in decagonal Al₇₂Ni₂₀Co₈, one of the best quasiperiodically ordered materials available today. We indeed find that significant point defects occur even for the highly-ordered quasicrystal, the localized distribution of which is well represented by the decagonal clusters located on the quasilattice with a length-scale of 2nm. Local disorder features appear to be significantly different between the clusters, but averaging them by concerning local symmetries of the Penrose tiling turns out to show a definite mirror symmetry, which seems to govern the global occurrence of the atomistic disorders. We are able to explain these remarkable disorder features as due to a phasonic perturbation of an (mostly) energetically stabilized Penrose-tile atomic structure.

Poster P-02

Title: Double-sided substitution sequences for pedestrians

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Abstract: Substitution sequences are useful models for quasiregular heterostructures which have recently attracted considerable interest [1]. Most algorithms for fabricating these structures are also based on substitution sequences. Sequences on \mathbb{N} or \mathbb{N}_0 , the positive or nonnegative integers, respectively, are well known (cf. [2]). Less popular are double-sided sequences, i.e. sequences on \mathbb{Z} , the set of all integers. Here I present simple ways to construct double-sided sequences and finite double-sided chains. Specifically, I deal with the double-sided versions of the Fibonacci, Thue-Morse, Rudin-Shapiro, paperfolding and period doubling sequences. Their spectral properties are the same as of their one-sided counterparts.

[1] F. Garca-Moliner, *Microelectronics Journal* **26** (2005) 870–875.

[2] On-Line Encyclopedia of Integer Sequences,

<http://www.research.att.com/~njas/sequences/Seis.html>

Poster P-03

Title: Aqueous Oxidation and characterisation of corrosion mechanisms of Al-Cr-(Cu)-Fe complex metallic alloys

Authors: •A. BENT¹, N.C. QUACH¹, E. URA^{1,2}, J.A. DEROSE¹, P. SCHMUTZ¹

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Abstract: Al-based Complex Metallic Alloys (CMA) show very attractive surface properties and peculiar aqueous oxidation stability[1] that render them promising materials in the field of corrosion resistance.

Very recently, the attention was focused on the study of corrosion behaviour of Al-Cr-(Cu)-Fe CMA. This was related to the availability of single phase samples prepared by powder sintering[2] or by Czochralski method from Al-rich solutions[3]. The two systems represent the testing grounds for a complete study on the corrosion mechanisms of those types of alloys. The sintered samples are found to be suitable for the characterisation of the thermodynamic electrochemical stability of the surface, while the defect-free, Czochralski grown ones, can be well exploited to study the resistance and mechanisms of localised attack (pitting corrosion).

In the presentation, characterisation of the thermodynamic electrochemical stability of powder sintered samples (Impedance Spectroscopy Analysis) will be reported together with the study on the electronic properties of the oxide film (Photoelectrochemistry and Mott-Schottky analysis). In addition to that, results will be shown on the localised corrosion susceptibility[4] of single phase defect-free monocrystalline Al₄(Cr,Fe) samples with Cr ranging between 12.5% and 18.5%. Comparisons with the behaviour of corrosion resistant materials that are currently exploited for industrial application will be reported.

[1] V. Fournée, M.-G. Barthés-Labrousse, J.-M. Dubois, Solid State Phenomena **138** (2008) 407.

[2] D. Veys, C. Rapin, X. Li, L. Aranda, V. Fournée, J.M. Dubois, J. Non-Cryst. Solids **347** (2004) 1.

[3] P. Gille, B. Bauer, Cryst. Res. Technol., **43** (2008) 1161.

[4] T. Suter, H. Bohni, Electrochim. Acta **42** (1997) 3275.

Poster P-04

Title: Thermal conductivity of Taylor phases $T\text{-Al}_{73}\text{Mn}_{27-x}\text{Pd}_x$

Authors: D. STANIĆ^{1,2}, P. POPČEVIĆ¹, I. SMILJANIĆ¹, Ž. BIHAR¹, A. BILUŠIĆ^{1,3}, I. BATISTIĆ⁴, •J. IVKOV¹, A. SMONTARA¹

Addresses: ¹Institute of Physics, Laboratory for the Study of Transport Problems, Bijenika 46, POB 304, HR-10000 Zagreb, Croatia ²Department of Physics, University of Osijek, Gajev trg 6, HR-31000 Osijek, Croatia ³Department of Physics, Faculty of Natural Sciences of the University of Split, Nikole Tesle 12, HR-21000 Split, Croatia ⁴Faculty Science, University of Zagreb, Bijenika c. 32, HR-10000 Zagreb, Croatia

Abstract: Thermal conductivity (κ) of complex-metallic-alloy (CMA) family of Taylor phases $T\text{-Al}_{73}\text{Mn}_{27-x}\text{Pd}_x$ ($x = 0, 2, 4, 6$) has been studied experimentally in the temperature interval from 2 K to 300 K. Behaviours in κ are typical for CMAs: relatively small in magnitude, change of slope at about 50 K and increase above 100 K. At room temperature the magnitude of κ for all the samples is between 2.7 W/mK and 3.7 W/mK, which is comparable to that of thermally insulating amorphous SiO₂ and Zr/YO₂ ceramics. Such a low thermal conductivity originates in complex structure aperiodic in short length scale, that leads to frequent electron scattering (i.e. to low electronic contribution to the thermal conductivity), while large lattice constant defines a small Brillouin zone that enhances *Umklapp* scattering of extended phonons. Above 100 K non-extended (localized) lattice vibrations are thermally excited, that gives a new heat carrying channel resulting in the typical increase of the thermal conductivity with temperature.

Poster P-05**Title:** Superspace groups of $(3 + d)$ -dimensional superspace**Authors:** H.T. STOKES¹, S. VAN SMAALEN², •B. CAMPBELL¹**Address:** ¹Department of Physics and Astronomy, Brigham Young University, Provo, Utah, USA²Laboratory of Crystallography, University of Bayreuth, Bayreuth, Germany**Abstract:** The symmetry of aperiodic crystals is described by superspace groups of $(3 + d)$ -dimensional space, where d is a positive integer that gives the number of independent modulation waves [1]. Superspace groups are a subset of the general space groups of space of dimension $n = 3 + d$, because point symmetries are restricted to point groups isomorphic to a point group in 3D space. Here, we discuss equivalence relations for superspace groups and efficient algorithms for equivalence testing and for the identification of superspace-group settings. We propose a table of superspace groups in $(3 + 2)$ and $(3 + 3)$ -dimensional superspace.[1] T. Janssen, A. Janner, A. Looijenga-Vos, P.M. De Wolff, in *International Tables for Crystallography Vol. C* (2006), ed. A.J.C. Wilson, pp. 907–955.**Poster P-06****Title:** Growth of large single-grain quasicrystal and approximant crystals in the Ag-In-Yb System**Authors:** C. CUI, •A.P. TSAI**Address:** Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan**Abstract:** Quasicrystals (QCs) are aperiodic solids that have long range order and rotational symmetries incompatible with conventional periodic lattice. Owing to the quasiperiodic atomic structure, these materials were expected to have inherent properties different from crystals. For detailed study on the intrinsic physical properties, large size high quality single-grain QCs and approximant (AP) crystals are highly desirable. The Ag-In-Yb icosahedral QC (*i*-QC) is considered to be a novel material for study on a single-grain QC [1]. First, the Ag-In-Yb *i*-QC is isostructural with the Cd-Yb *i*-QC, whose atomic structure has recently been determined and can be described as an aperiodic arrangement of rhombic triacontahedral clusters which contain 94% of the total atoms in the crystal, being different from most Al-based icosahedral *i*-QCs [2]. Second, the Ag-In-Yb is easy to handle because it is stable in air and it doesn't contain elements of high vapor pressure or toxicity. Third, two AP crystals which are ordinary crystals closely related to the *i*-QC in chemical composition and the local atomic structure, exist as stable phases.

In our experiment, by carefully designing the temperature program, growth rate and composition we successfully synthesized centimeter-size single-grain *i*-QC by the Bridgman method. It was also confirmed that the growth of single-grain *i*-QC was sensitive to the starting composition, especially the content of Yb, which is limited within 15-16 at.%. However, this method is not suitable for synthesizing large single-grain AP crystals due to the peritectic reaction. Then, we used a self-flux method, in which large single-grain Ag-In-Yb *i*-QC, 2/1 and 1/1 AP crystals have been successfully synthesized from the indium-rich melt. These crystals show typical natural facets, i.e., 5-fold and 3-fold planes in the single-grain quasicrystal, (100) and (110) planes in the 1/1 approximant crystal, and (111) planes in the 2/1 approximant crystal. These planes are considered to be the typical thermostable planes in the *i*-QC and AP crystals. We believe these single-grain *i*-QCs and AP crystals will be very useful for the study of intrinsic physical properties as well as surface properties.

[1] J.Q. Guo and A.P. Tsai, *Phil. Mag. Lett.* **88** (2002) 349.[2] H. Takakura, C.P. Gomez, A. Yamamoto, M. de Boissieu, A.P. Tsai, *Nature Materials* **6** (2007) 58.

Poster P-07

Title: Electronic structure of the $\text{Al}_{13}\text{Co}_4$ complex metallic alloy

Authors: TH. DENIOZOU¹, K. HORN¹, W. THEIS², J.M. CHESNEY³, A. BOSTWICK³, E. ROTENBERG³, K.V. EMTSEV⁴, TH. SEYLLER⁴, R. ADDOU⁵, V. FOURNÉE⁵, J. LEDIEU⁵, R. WIDMER⁶, Y. GRIN⁷, M. HEGGEN⁸, M. FEUERBACHER⁸

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Abstract: The investigation of periodic approximant phases may help to understand the physical properties of their close relatives, the quasicrystalline alloys, in particular with respect to the electronic structure which leads to the formation of the latter. Here we report angle-resolved photoemission studies of the complex metallic alloy $\text{Al}_{13}\text{Co}_4$ which is an approximant of the decagonal Al-Ni-Co quasicrystal. We use the tenfold symmetric $\text{Al}_{13}\text{Co}_4(100)$ surface to examine the electronic states in the valence band, and show that the density of states at the Fermi level is dominated by s-p-derived Al and Co electronic states, while the d-derived states are removed from this region, in agreement with calculations. The observed constant energy photoemission intensity patterns can be interpreted in terms of s-p states emanating from different reciprocal lattice vectors to give a consistent picture of the Fermi surface of this material.

Poster P-08

Title: The Al-Cu-Ta family of complex metallic alloys

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Abstract: Complex metallic alloys (CMAs) are intermetallic compounds with a huge degree of complexity in their crystal structure compared to their seemingly simple composition. They feature big unit cell volumes that can hold hundreds or thousands of atoms.

We already reported the series of compounds $\text{Al}_{63.6}\text{Ta}_{36.4}$, $\text{Al}_{56.6}\text{Cu}_{3.9}\text{Ta}_{39.5}$ and $\text{Al}_{55.4}\text{Cu}_{5.4}\text{Ta}_{39.1}$ as cluster-based structures [1,2]. All of them are found to crystallize in the $F\bar{4}3m$ spacegroup and they exhibit lattice constants of approximately $a = 19 \text{ \AA}$, 45 \AA and 71 \AA , respectively. The latter structure is the intermetallic phase with the by far largest unit cell reported to date, which contains over 23 000 atoms. The thorough discussion of the constituting clusters reveals the high degree of commonness these three structures possess [2]. Now, a complementary aspect will be discussed.

The periodic approach does justice to a rather diverse diffraction pattern that cannot clearly be distinguished into a set of strong main reflections and a set of weaker satellites. However, there are some strong intensities, that appear in all three diffraction patterns. This corresponds to their common average structure which can be regarded as a cubic Laves phase with a unit cell parameter $a = 6.5 \text{ \AA}$. The three mentioned structures can therefore be interpreted as 3-fold, 7-fold and 11-fold superstructures, respectively. The transformation into a representation as a modulated structure leads to a cubic and thus $(3 + 3)$ -dimensional supergroup. The description of these crystal structures as modulated structures will be presented. The systematics which can be expressed through this formalism are examined to better understand the structure and structure-building mechanisms of the Al-Cu-Ta family.

[1] T. Weber *et al.*, Acta Cryst. B **65** 308–317.

[2] M. Conrad *et al.*, Acta Cryst. B **65** 318–325.

Poster P-09

Title: Superspace model for the terrace-like structures in the Bi-Sr-Fe-O system.

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Abstract: Two members of the Bi-Sr-Fe-O system, ($x = 3/20, 7/47$ of the general $\text{Bi}_{2x}\text{Sr}_{3x}\text{Fe}_{1-5x}\text{O}_{1+2x}$), have been re-analyzed within the superspace framework. These monoclinic terrace (or stair-like) structures are built up of $[\text{Bi}_2\text{Sr}_3\text{Fe}_2\text{O}_9]$ 2212-type slices interconnected through $[\text{Bi}_2\text{Sr}_3\text{FeO}_8]_\infty$ blocks [1]. The existence of a common and simple average structure suggests the existence of a single superspace model with a single superspace group and modulation wave-vector $q = (\frac{1-3x}{2}, 0, -2x)$, that can be used to describe and refine the structures in a more efficient way.

The existence of several other terrace members, synthesized as powder samples, were frequently reported from HREM images in the Bi-Sr-Fe-O or Bi-Sr-Cu-O systems [2]. However, the complexity of these compounds compromises the accurate structure determination using X-ray powder diffraction. The achievement of a superspace model is a helpful tool to understand the chemical mechanisms associated with the formation of terrace phases.

A single independent continuous atomic domain has been used to represent the cations (Bi-Sr-Fe), divided into different regions corresponding to the different elements, and two crenel-like O atomic domains. Despite their strong anharmonicity, a striking invariance of the form of the atomic domains in the two compounds is evidenced, supporting the soundness of the model. The refinements also show the usefulness of the Legendre polynomials, recently introduced in JANA2006 [3], to describe the displacive modulations of crenel-like domains of small size.

[1] M. Allix *et al.*, J. Solid State Chem. **177** (2004) 3187–3196; M. Hervieu *et al.*, J. Solid State Chem. **129** (1997) 214–222; O. Pérez *et al.*, Phys. Rev. B **56** (1997) 5662–5672.

[2] M. Hervieu *et al.*, J. Solid State Chem. **118** (1995) 357.

[3] Petříček *et al.*, Jana2006. The crystallographic computing system. Institute of Physics, Praha, Czech Republic (2006).

Poster P-10

Title: Growth of quasicrystals by a relaxation process

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Abstract: Tilings are often used as a toy model for quasicrystals, with the ground states corresponding to the tilings satisfying some local properties (*matching rules*). In this context, a challenging problem is to provide a theory for quasicrystals growth. One of the proposed theories is the *relaxation process* [1]. One assumes that the entropy of a tiling increases with the number of tilings which can be formed with the same tiles, while its energy is proportional to the ratio of satisfied matching rules. Then, by starting from an entropically stabilized tiling at high temperature and by decreasing the temperature, the phason flips which decrease (resp. increase) the energy would become more and more favoured (resp. inhibited). Ideally, the tiling eventually satisfies all the matching rules, thus shows a quasicrystalline structure. The purpose of this talk is to describe a stochastic process inspired by this and to discuss convergence rates towards ground states. We present experimental results for the Penrose rhomb tiling, which surprisingly shows a rather fast convergence [2]. We also present some theoretical results in a simpler case (co-dimension one tilings).

[1] C. Janot, Oxford University Press (1992) p. 356.

[2] See <http://www.lif.univ-mrs.fr/~fernique/stochasflip/animation.html>

Poster P-11**Title:** *Ab initio* structure solution of quasicrystals by iterative phase-retrieval algorithms**Authors:** •F. FLEISCHER, TH. WEBER, W. STEURER**Address:** Laboratory of Crystallography, ETH Zurich, Zurich, Switzerland**Abstract:** The extension of Fourier recycling techniques to arbitrary dimensions [1,2] provides an easy access to quasiperiodic structures. The structure solution of quasicrystals in higher dimensions leads to the reconstruction of geometrical objects, the occupation domains. Algorithms, like low density elimination and charge-flipping were successfully applied to solve quasiperiodic structures [e.g. 1,3]. However, their working principle is unsatisfactory understood and investigated.

In this contribution, we present a comprehensive study on the charge-flipping and low density elimination algorithm applied on quasicrystals. Systematic performance tests clarify the strengths and weaknesses of the algorithms. Since the first iteration step of such an algorithm is initialized by random phases, the resulting phased data sets differ slightly. Statistical investigations on several solutions allow distinguishing between reliable and random retrieved phases. Furthermore, the definition of a figure of merit provides a quantitative estimate of the resulting phase set. We used synthetic diffraction data of quasicrystals to perform quality tests. Finally, we propose an optimized strategy for handling experimental data. The improvement on the quality of resulting electron density maps will be shown on the example of decagonal quasicrystals.

[1] H. Takakura, M. Shiono, T.J. Sato, A. Yamamoto, A.P. Tsai, *Phys. Rev. Lett.* **86** (2001) 236–239.

[2] L. Palatinus, *Acta Cryst.* **60** (2004) 604–610.

[3] S. Katrych, T. Weber, M. Kobas, L. Massüger, L. Palatinus, G. Chapuis, W. Steurer, *J. Alloys Compd.* **428** (2007) 164–172.

Poster P-12**Title:** A stone-inflation for square triangle tilings**Author:** D. FRETTLÖH**Address:** Univ. Bielefeld, Germany**Abstract:** Square triangle tilings are relevant models for quasicrystals showing 12-fold dihedral symmetry. Several families of square triangle tilings can be found in the literature, and several construction methods for them are known. Nevertheless, the most frequent construction methods for nonperiodic tilings are difficult to apply to square triangle tilings. (a) Substitution rules: It is hard to give a substitution rule (in the sense of: each tile of the same type is substituted by the same patch) for square triangle tilings. (b) Cut and project schemes: It is conjectured that the window (= acceptance domain = atomic surface) of a 12-fold symmetric square triangle tiling is always of fractal nature.

We present a certain substitution for (statistical) 12-fold symmetric square triangle tilings. This substitution rule is a stone-inflation, that is, a square is indeed mapped to a square patch, and a triangle is mapped to a triangular patch. This rule is a variant of Martin Schlottmann's square triangle substitution (which is not a stone-inflation). Moreover, we approximate the window, and discuss its role as a fractal fundamental domain of the hexagonal lattice.

Poster P-13**Title:** MLD Relations of Pisot Substitution Tilings**Author:** F. GÄHLER**Address:** Faculty of Mathematics, Bielefeld University, D-33501 Bielefeld, Germany

Abstract: We consider 1-dimensional, unimodular Pisot substitution tilings with three intervals, and discuss conditions under which pairs of such tilings are locally isomorphic (LI), or mutually locally derivable (MLD). For this purpose, we regard the substitutions as homomorphisms of the underlying free group with three generators. Then, if two substitutions are conjugated by an inner automorphism of the free group, the two tilings are LI, and a conjugating outer automorphism between two substitutions can often be used to prove that the two tilings are MLD. We present several examples illustrating the different phenomena that can occur in this context. In particular, we show how two substitution tilings can be MLD even if their substitution matrices are not equal, but only conjugate in $GL(n, \mathbb{Z})$. We also illustrate how the (in our case fractal) windows of MLD tilings can be reconstructed from each other, and discuss how the conjugating group automorphism affects the substitution generating the window boundaries.

Poster P-14**Title:** CSLs of the root lattice A_4 **Authors:** M. HEUER¹, P. ZEINER¹**Address:** ¹Department of Mathematics and Statistics, The Open University, Milton Keynes, UK
²Fakultät für Mathematik, Universität Bielefeld, Germany

Abstract: Recently, the group of coincidence isometries of the root lattice A_4 has been determined providing a classification of these isometries with respect to their coincidence indices. A more difficult task is the classification of all CSLs, since different coincidence isometries may generate the same CSL. In contrast to the typical examples in dimensions $d \leq 3$, where coincidence isometries generating the same CSL can only differ by a symmetry operation, the situation is more involved in 4 dimensions. Here, we find coincidence isometries that are not related by a symmetry operation but nevertheless give rise to the same CSL.

We show how the classification of CSLs can be obtained by making use of the icosian ring and provide explicit criteria for two isometries to generate the same CSL. Moreover, we determine the number of CSLs of a given index and encapsulate the result in a Dirichlet series as generating function.

Poster P-15**Title:** Diffraction intensity and photonic band gap**Author:** H.-C. JEONG**Address:** Department of Physics, Sejong University, Gwangjin-gu, Seoul 143-747, Korea

Abstract: Optimized structures for photonic crystals are investigated in terms of their diffraction intensities. We study optimal structures composed of materials with two different dielectric constants. By comparing these optimal photonic structures with optimal density structures which give rise to the maximal diffraction intensity for given total mass, we obtained the relationship between the dielectric constant contrasts and the density contrasts in one-dimensional (1D) structures. Our finding may provide a new method to predict the 3D optimal band-gap structures through diffraction intensity calculation which requires much less numerical costs.

Poster P-16

Title: Characterization of quasicrystalline Al-Cu-Fe nanoclusters as the catalyst for the synthesis of carbon nanotubes

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Abstract: Quasicrystalline (QC) Al-Cu-Fe nanoclusters as the catalyst for the synthesis of carbon nanotubes (CNTs) have been studied as shown in our previous paper [1]. It was shown that armchair-type (i.e., metallic) CNTs are preferentially synthesized by using QC nanoclusters as catalysts in catalytic chemical vapor deposition. It was postulated that the structure of QC nanoclusters with fivefold symmetry plays an important role in the nucleation of a CNT cap with specific six-pentagons-configuration, which gives rise to the selective synthesis of, e.g., an armchair-CNT (9,9). To verify this hypothesis, in this study the size and structure of QC nanoclusters were investigated by using transmission electron microscopy and electron diffraction (ED) as well as X-ray diffraction.

As a result, the average diameter of nanoclusters is ~ 4 nm, ranging from 1 nm to 10 nm, which seems to correlate with the diameter distribution of CNTs. The shapes are generally faceted-polyhedra. ED patterns could be attributed to the icosahedral-Al-Cu-Fe and alpha-alumina. It is also found that multi-walled CNTs (MWNTs) were synthesized successfully using *i*-AlPdRe and *d*-AlCoNi bulk samples as catalysts. It implies that larger QC nanoclusters have a significant catalytic activity for the synthesis of MWNTs.

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Poster P-17

Title: Real space structure refinement of the basic Ni-rich decagonal Al-Ni-Co phase

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Abstract: We present a real space structure refinement of the basic Ni-rich decagonal Al-Ni-Co phase based on a diffraction data set, without referring to the five-dimensional properties of decagonal quasicrystals. The structure factor, which was used for the modelling process, was calculated using a statistical method [2], which allows a purely 3-dimensional, real space optimization of a quasicrystalline structure. Decagonal Al-Ni-Co quasicrystals are known to consist of aperiodic planes stacked periodically along the quasi-tenfold axis (*c*-axis). There are two planes within one period of the *c* axis. We assumed, that the projection of these two planes along the *c*-axis results in rhombic Penrose tiling. The rhombuses are divided three times with obedience to the inflation rules. The idealized positions of atoms are the points of subsequent divisions. We also put several atoms in the positions of the fourth division to fulfil the density restriction. There are 70 atoms decorating our structure units. They are divided into groups according to the overlapping rules for kite-clusters [3]. For each group a shift from ideal position, anisotropic Debye-Waller factor, occupation probability and concentration of TM atom are refined. We obtained *R*-factor at the level of 12% and *R_w*-factor of 6%. The resulting structure has the chemical composition, point density and overall density values very close to the experimental ones. The optimization was performed on a set of 2767 diffraction peaks taken by a 4 four-circle diffractometer at beamline D3, HASYLAB [1].

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[3] M. Duda, B. Kozakowski, J. Wolny, J. Non-Crystalline Solids **353** (2007) 2500–2505.

Poster P-18**Title:** Configuration energy analysis of β -Mg₂Al₃ cluster structure**Authors:** •B. LABNO, L. PYTLIK, J. ADAMOWSKI, J. WOLNY, M. DUDA**Address:** Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland

Abstract: The problem of stability of β -Mg₂Al₃ clusters has been studied with the use of effective potential obtained from ab-initio calculations [1]. The total potential energy has been calculated for different possible β -Mg₂Al₃ clusters in order to find the optimal ones. The computation was started from the cluster located at the 8(b) site consisting of 72 partially occupied, overlapping atomic sites, as determined by diffraction data [1]. Therefore, 2^{72} possible configurations would have to be generated and compared. The search of the equilibrium configurations has been carried out by scanning the configuration subsets with use of a divide and conquer computation scheme. It has been found that for the effective number of atoms exceeding 17 the configuration energy increases. The majority of the optimal configurations has been obtained for the clusters with 16 or 17 atoms. In the second stage, the other partially occupied sites have been added, which form the interfaces between the previously considered clusters. Next, the fully occupied atomic sites have been included, which form an external framework which stabilizes the entire cluster configuration. The energy optimization performed for all the atoms allowed us to determine several configurations with the energy close to the minimum. Up to this stage, all the atoms were allowed to take only the discrete set of positions in accordance with the space group determined by diffraction. In the final stage, the configurations have been tuned by giving the atoms freedom to move continuously in 3D space by using the simulated annealing algorithm. The results obtained have been used to create the more complex structures by constructing combinations of neighbouring low energy atomic clusters, which later subjected to the energy optimization. For such structures the configurational entropy has been calculated the as a function of the total potential energy. The radial and angular distributions have been also determined for atoms in clusters, which reveal the shell structure of local configurations. The obtained atomic compositions and the total potential energy per atom exhibit the expected asymptotic behaviour as a function of the number of atoms.

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Poster P-19

Title: Crystal structure of $C_{64}H_{78}Cl_2N_6O_{56}P_1Ru_2W_{12}$ with “incommensurate” point group

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Abstract: Usually the term “incommensurate” is applied to composite crystals that may be described as being composed of a finite number of subsystems, each with its own space-group symmetry. The lattices of these subsystems may be mutually incommensurate. In the special case, the subsystems may be mutually commensurate, or in other words, there are three basis vectors such that vectors are integral with definite accuracy by linear combinations of basic vectors of all subsystem lattices [1]. However, even in the last case, in the course of the practical work of structure refinement, sometimes it is possible and easier to consider such structure as incommensurate without applying a space group of superstructure, because it may have a very large unit cell.

Space-group symmetry of subsystems can be different not only by their translational elements but also by elements of their point groups. As an example we present here the results of solution and refinement of the composite molecular crystal structure of polyoxometalate $C_{64}H_{78}Cl_2N_6O_{56}P_1Ru_2W_{12}$. Its unit cell comprises one alpha-Keggin anion $PW_{12}O_{40}^{3-}$, two organometallic molecules $C_{30}H_{36}Cl_1N_2O_5Ru_1$ (complex 2), and as solvents – two molecules of acetonitrile and at least 6 disordered water molecules represented by their oxygen atoms. The structure is approximately P1bar as the large complex 2 molecules are related with high accuracy by an inversion center which could be considered as the origin of a P1bar cell, but which does not exactly coincide with the center of Keggin anion (near Phosphorus position). The small shift of the Keggin anion center breaks the inversion symmetry. The structure was solved and refined in space group P1 with the application of restrains in order to avoid a degeneration of minimizing functional because of higher symmetry of complexes 2. From other point, this structure may be considered as composed of different subsystems with their own space-group symmetry and treated by the way which is similar to processing of incommensurate structures.

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Poster P-20

Title: Applications of the maximum entropy method to incommensurate modulated crystal $Cr_2P_2O_7$

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Abstract: One of the applications of the Maximum Entropy Method (MEM) in crystallography is the reconstruction of the electron density from phased structure factors. In aperiodic crystallography the MEM can be used to determine the shapes of the modulation functions. Modulation functions are usually determined by structure refinements employing the superspace formalism. The true modulation functions are not necessarily obtained by this method, because only a limited number of parameters can be refined, while additional parameters would lead to numerical dependencies among them. MEM is a model-independent tool to obtain the most probable electron density in superspace. In the present work, the MEM is applied to experimental data of $Cr_2P_2O_7$ [1]. A new structure model and the shapes of modulation functions are obtained from the analysis of the MEM derived electron density map. Disorder of the structure is confirmed and the positional modulation functions of atoms at the disorder range are derived.

[1] L. Palatinus, M. Dušek, R. Glaum, B. El Bali, *Acta Crystallographica Section B* **62** (2006) 556–566.

Poster P-21**Title:** Studies on phason flips by kinetic Monte Carlo simulations**Authors:** •H. LIPP, H.-R. TREBIN**Address:** Institut für Theoretische und Angewandte Physik, University of Stuttgart, Stuttgart, Germany**Abstract:** Neutron scattering experiments [1] indicate that atoms in quasicrystals perform flips between split positions with typical time scales of picoseconds. On the other hand, Edagawa et al. have presented HRTEM images [2], where bright spots are flipping with periods of seconds or even minutes.

To explain this apparent discrepancy, we start from a structure model for d-Al-Cu-Co of Zeger et al. [3], where a ring of ten atoms can perform a jump by four consecutive single atom flips. By applying kinetic Monte Carlo simulations [4], we study how these collective flips, which occur in the different layers of the d-phase can lead to flips detectable by HRTEM on much lower frequency scales.

[1] G. Coddens, S. Lyonnard, Y. Calvayrac, Phys. Rev. Lett. **78** (1997) 4209.[2] K. Edagawa, K. Suzuki, S. Takeuchi, Phys. Rev. Lett. **85** (2000) 1674.[3] G. Zeger, H.-R. Trebin, Phys. Rev. B **54** (1996) R720.[4] A.B. Bortz, M.H. Kalos, J.L. Lebowitz, J. Comput. Phys. **17** (1975) 10.**Poster P-22****Title:** Electrical resistivity of Al-Pd-Re quasicrystal prepared by spark plasma sintering method**Authors:** •T. MORI¹, Y. WAKUDA¹, R. TAMURA¹, K. NISHIO¹, K. TOKIWA²**Addresses:** ¹Dept. of Mater. Sci. & Tech., Tokyo University of Science, Chiba 278-8510, Japan²Dept. of Appl. Elec., Tokyo University of Science, Chiba 278-8510, Japan**Abstract:** Poly-grained icosahedral Al-Pd-Re quasicrystal has been known to exhibit an insulating behavior at low temperatures ($\rho_{300\text{K}} \approx 16000 \mu\Omega \text{ cm}$, $\rho_{4.2\text{K}}/\rho_{300\text{K}} > 70$) [1] for a specific alloy composition of $\text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5}$ [2]. However, there has been a debate that this insulating property comes from the porous microstructure with narrow oxidized conduction paths [3]. Therefore, in this study, in order to avoid the formation of the porous microstructure we prepared $\text{Al}_{70.5}\text{Pd}_{21}\text{Re}_{8.5}$ using Spark Plasma Sintering (SPS) method that allows us to prepare fully-density and homogeneous samples.

It has been found that the sample prepared by SPS exhibits insulating properties such as high electrical resistivity ($\rho_{300\text{K}} \approx 5000 \mu\Omega \text{ cm}$) and a large negative temperature coefficient of the resistivity ($\rho_{4.2\text{K}}/\rho_{300\text{K}} \approx 12$), which suggests that the insulating behavior of the Al-Pd-Re quasicrystal at low temperatures is an intrinsic property to the quasicrystal.

[1] F.S. Pierce, Q. Guo, S.J. Poon, Phys. Rev. Lett. **73** (1994) 2220.[2] H. Akiyama *et al.*, Jpn. J. Appl. Phys. **32** (1993) 1003.[3] J. Dolinsek *et al.*, Phys. Rev. B **74** (2006) 134201.

Poster P-23**Title:** Low temperature phase transitions of Cd_6M ($M=Nd,Gd,Tb$) approximants**Authors:** •M. MURAKI¹, K. NISHIMOTO¹, T. YAMADA¹, R. TAMURA¹, Y. MURO², K. MOTOYA²**Addresses:** ¹Dept. Mater. Sci. & Tech., Tokyo University of Science, Noda, Chiba, Japan²Dept. Phys., Tokyo University of Science, Noda, Chiba, Japan**Abstract:** Cd_6Yb and Cd_6Ca approximants, which have a Tsai-type cluster as a structural unit, was found to exhibit a structural phase transition at 110K and 100K, respectively. The transitions were attributed to ordering of the disordered tetrahedron at the center of the Tsai-type cluster [1,2]. Such a low-temperature phase transition has also been found in other C_6M ($M=Rare\ earth$) approximants. However, the detail of the phase transition has not been well investigated for Cd_6M ($M=Nd,Gd,Tb$). Therefore, in this study we have studied the phase transitions of Cd_6M ($M=Nd,Gd,Tb$) by electrical resistivity and specific heat measurements etc. As a result, Cd_6M ($M=Nd,Gd,Tb$) are found to exhibit a peak in the specific heat at about 146K, 185K, 170K, which indicates a change of the entropy due to the phase transition. The entropy changes are attributed to an ordering of the tetrahedron located at the center of the Tsai-type cluster and the transition entropies are estimated to be $0.49k_B$, $0.30k_B$ and $0.43k_B$ per unit cell for Cd_6M ($M=Nd,Gd,Tb$), respectively. These values are smaller than the entropies obtained for Cd_6Yb and Cd_6Ca , which might suggest that the orientation of the tetrahedron is not fully ordered below T_c for these approximants.[1] R. Tamura *et al.*, Jpn. J. Appl. Phys. **41** (2002) L524.[2] R. Tamura *et al.*, J. Non-Cryst. Solids **334&335** (2004) 173.**Poster P-24****Title:** Structural characterization of Bi deposited on the five-fold surface of icosahedral Al-Pd-Mn**Authors:** •T.C.Q. NOAKES¹, P. BAILEY¹, R. MCGRATH², J.A. SMERDON², L. LEUNG², C.F. MCCONVILLE³, M. WALKER³, M. BROWN³, M. DRAXLER⁴, A.R. ROSS⁵, T.A. LOGRASSO⁵**Addresses:** ¹STFC Daresbury Laboratory, Daresbury, Warrington, Cheshire, WA4 4AD, UK²Surface Science Research Centre, University of Liverpool, Liverpool, L69 3GH, UK³Department of Physics, University of Warwick, Coventry, CV4 7AL, UK⁴Institute of Experimental Physics, Johannes Kepler University Linz, A-4040 Linz, Austria⁵Ames Laboratory, Iowa State University, Ames, IA 50011, USA**Abstract:** Recent work on the growth of thin metal films on quasicrystalline substrates has indicated the formation of so-called 'magic height' islands for both Ag on *i*-AlPdMn and Bi on *i*-AlCuFe [1]. The preferred island height of 4ML is thought to arise as a result of quantum size effects, which lead to enhanced stability at these dimensions and indeed for Ag on *i*-AlPdMn (and *d*-AlNiCo) quantum well states have been observed using low temperature photoemission [2]. This presentation reports a study of Bi deposition on *i*-AlPdMn using medium energy ion scattering to characterise cluster size and the structural arrangement within the clusters. In addition, data was taken for annealed surfaces where the Bi clusters desorb to leave a single aperiodic monolayer of material at the surface. Energy spectra from the Bi islands was seen to be consistent with a single monolayer covered with 4 ML islands for coverages of both 1.5 ML and 3 ML. In addition, the angular dependence of the Bi scattered ion intensity has been tested against models of both rhombohedral Bi and a distorted structure reported for Bi clusters formed on Si(111) [3]. In the case of the aperiodic Bi monolayer, the angular spectra have also been tested against structural models, including a recent theoretical prediction [4].[1] V. Fournée *et al.*, Phys. Rev. Lett. **95** (2005) 155504.[2] P. Moras *et al.*, Phys. Rev. B **74** (2006) 121405(R).[3] T. Nagao *et al.*, Phys. Rev. Lett. **93** (2004) 105501.[4] M. Krajčí, J. Hafner, Phys. Rev. B **71** (2005) 184207.

Poster P-25

Title: First-principles study for effect of lattice defects on the order-disorder transition in Cd-Ca and Zn-Sc cubic crystalline approximants

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Abstract: Cd₆Ca and Zn₆Sc, which are 1/1 cubic approximants of binary quasicrystals Cd_{5.7}Yb/Ca and ternary ones Zn-M-Sc (M=Mg, Fe, Co, Ni, . . .), exhibit order-disorder transitions at low temperatures about 100 K. The crystal structure of the approximants are described using four-layered atomic shells called Tsai-clusters. The order-disorder transition is considered to be a result of an orientational change of tetrahedral atomic shells located at the center of the Tsai-cluster. Recently, Yamada and Tamura found the transition is sensitively affected by lattice defects.

In this study, effect of lattice defects on the transition is investigated using the first-principles density functional method with plane-wave basis sets. A cubic cell including 168 atoms (two Tsai-clusters) is used as a unit cell. Several atomic sites are replaced by a vacancy and all of the rest are relaxed according to evaluated forces at each calculation step. Significant displacements in the tetrahedral core are found even in cases where the vacancy is introduced in the outermost shell. Results of atomic substitutions will also be presented.

Poster P-26

Title: Adsorption of Sb on the i-AgInYb quasicrystal

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Abstract: AgInYb is isostructural to the binary quasicrystal CdYb [1]. This trimetallic quasicrystal is important in further understanding of the binary system. Several techniques have been employed in the attempt to discover the surface structure of this quasicrystal including Scanning Tunneling Microscopy (STM), Low Electron Energy Diffraction (LEED), and X-ray Photo Spectroscopy (XPS). One technique that can be employed to probe the surface structure is the atomic deposition of certain elements that bond well to particular species that exist on the targets surface. One such element, Antimony, is a candidate for exploring the AgInYb system. Antimony has been grown until there is one complete monolayer on the surface. STM shows that the Sb atoms form a 1:1 bond with the Yb atoms of the substrate. This monolayer has the exact same structure as the substrate it has been grown upon and highlights the position of the Yb atoms. This layer exhibits the same long range ordering as its substrate with no periodicity, giving rise to a quasicrystalline formation.

[1] J. Guo and A.P. Tsai, *Phil. Mag. Lett.* **82** (2002) 349.

[2] H.R. Sharma, M. Shimoda, K. Sagisaka, H. Takakura, J.A. Smerdon, P.J. Nugent, R. McGrath, S. Ohhashi, A.P. Tsai, submitted.

Poster P-27**Title:** Beyond the Bärnighausen tree with superspace**Authors:** •I. ORLOV, G. CHAPUIS**Address:** Laboratoire de Cristallographie, Le Cubotron/BSP, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland**Abstract:** During phase transitions and solid state reactions which result in products of lower symmetry, the higher symmetry of the starting material is indirectly preserved by the formation of oriented domains. This concept formulated by Bärnighausen [1] renders itself useful for uncovering hidden symmetry relations between seemingly different structures. The same is also true for the superspace formalism which was introduced for the description of aperiodic structures. Using this formalism for the unified description of sets of commensurate structures requires an unambiguous understanding of how symmetry of a 3-dimensional structure may be inherited from the symmetry of a higher-dimensional one. Although the 2D scanning groups resulting from 3D groups has been thoroughly described, the equivalent for (3+1)D and 3D groups was missing for a long time. The most apparent reason for this absence is the fact that related crystal structures often have different 3D space groups and the relationships between them become visible only in higher dimensional space. These relations were only partially known until Orlov et al. [2] summarized the hyperplane t cuts of (3+1)D symmetry elements and constructed a complete network relating (3+1)- and the corresponding 3-dimensional space groups derived by rational cuts. A database containing the complete set of data for (3+1) to 3D group relations has been included in the online version of International Tables for Crystallography in 2008 [3].

This talk gives insight into the extension of the Bärnighausen trees by using the superspace concept. Not only all the possible structure derivatives can be derived from a single model including the space group symmetry but also the lattice constants can be predicted. The use of symmetry relationships derived from superspace group considerations will be presented with a study of some well known families of compounds. With that approach it would be interesting to find out what is the minimal number of crystal-structure types one needs to describe crystalline structures?

[1] H. Bärnighausen, *MATCH, Commun. Math. Chem.* **9** (1980) 139–175.

[2] I. Orlov, L. Palatinus, G. Chapuis, *J. Appl. Cryst.* **41** (2008) 1182–1186.

[3] International Tables Online: Superspace Finder, <http://it.iucr.org/resources/finder/>

Poster P-28**Title:** Investigation of Mg-Zn-Dy phase diagram in the vicinity of the decagonal composition**Authors:** •T. ORS, F. FLEISCHER, F. ALBERTINI, A.T. BAIER, W. STEURER**Address:** Laboratory of Crystallography, Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland**Abstract:** Mg-Zn-R (R = rare-earth and Y) alloys are important systems for quasicrystal research as the only non-Al bearing systems that are reported to have a decagonal phase [1] belong to this group. In this study, Mg-Zn-Dy system is investigated in the vicinity of the decagonal composition ($Zn_{58}Mg_{40}Dy_2$ [2]) to check the composition-dependent stability and the grain growth behavior. The alloys were prepared by induction melting and annealed at different temperatures. X-ray diffraction results showed that the icosahedral phase was dominant in the alloys which have a Dy content of 5 at.% or more. For lower Dy contents, however, either Dy dissolved $MgZn_2$ is found to coexist with a phase similar to the $(Ga,Zn)_{171.43}Mg_{100.57}$ phase [3] or a hexagonal phase with $a = 14.55 \text{ \AA}$ and $c = 8.680 \text{ \AA}$ similar to $Zn_{65.2}Mg_{28.3}Sm_{6.5}$ [4] forms with an additional phase. The existence of these phases and their compositions are also checked by the electron microprobe analysis method. Also, grain growth behavior was observed with optical microscopy and scanning electron microscopy techniques. Further research will focus on specifying the composition of the decagonal phase and growing decagonal quasicrystals that are large enough to be examined by single crystal X-ray diffraction.

[1] T.J. Sato, E. Abe, A.P. Tsai, *Jpn. J. Appl. Phys.* **36** (1997) 1038–1039.

[2] T.J. Sato, E. Abe, A.P. Tsai, *Phil. Mag. Lett.* **77** (1998) 213–219.

[3] G. Kreiner, *J. Alloys Comp.* **338** (2002) 261–273.

[4] K. Sugiyama, K. Yasuda, T. Ohsuna, K. Hiraga, *Z. Kristallogr.* **213** (1998) 537–543.

Poster P-29**Title:** Tailor-made sevenfold approximants: ab-initio investigations on formation and stability**Authors:** •H. ORSINI-ROSENBERG, D. JUNG, W. STEURER**Address:** Laboratory of Crystallography, ETH Zurich, Zurich, Switzerland**Abstract:** Sevenfold symmetry is the lowest symmetry not yet observed in quasicrystals. However, there are several strong hints that indicate the existence of heptagonal quasicrystals (QCs) [1]. In rare earth transition metal borides and borocarbides, several layered structure types can be understood as approximants of two-dimensional sevenfold QCs. They consist of the rhomb unit tiles from the planar heptagonal tiling. However, all of the known stable structures contain only two of the three rhomb tiles necessary. Finding a stable approximant containing all three heptagonal unit tiles is a crucial step on the way towards heptagonal quasicrystals.Starting from the two most promising structure types, ScB_2C_2 (consisting of the “fat” and “thin” rhomb) and YB_2C (“middle” and “thin” rhomb), new approximants were designed. The resulting structures were assembled from three-tile supertiles taken from the two starting structures, and contain all three rhomb types.

Using VASP [2], we performed ab-initio calculations on different combinations of rare earth elements in these structures. The chemical stability of mixed crystal series, as well as reaction equations for future synthesis, were calculated. In addition, molecular dynamics simulations at elevated temperatures were conducted in order to understand the dynamics of the systems. From our results we will conclude which systems are most suitable for future experimental research.

[1] W. Steurer, Boron-based quasicrystals with sevenfold symmetry, *Phil. Mag.* **87** (2007) 2707–2712.[2] “Vienna Ab-initio Simulation Package”; G. Kresse, J. Furthmüller, *Phys. Rev. B* **54** (1996) 11169.**Poster P-30****Title:** A comparative study of omnidirectional mirrors based on aperiodic porous silicon multilayers**Authors:** •A. PALAVICINI¹, C. WANG²**Addresses:** ¹Departamento de Fisica, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico, Apartado Postal 70-542, 04510, D.F., Mexico ²Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Apartado Postal 70-360, 04510, D.F., Mexico**Abstract:** By using the transfer matrix method [1], we calculate the reflectance of aperiodic porous silicon multilayers, such as Fibonacci and Thue-Morse sequences. The results for all directions of light incidence and a wide range of wavelengths are compared with those obtained from the periodic case. Some advantages and disadvantages of aperiodic omnidirectional mirrors are discussed. These results could be important for the design of photonic devices. In addition, we have fabricated aperiodic multilayers of porous silicon, by etching a crystalline silicon wafer in a solution of hydrofluoric acid and alternating porous silicon layers with high and low refractive indices. Porous silicon is a nanostructured material and exhibits efficient photo- and electroluminescence in the visible spectrum at room temperature [2], as well as a tunable refractive index mainly determined by its porosity. Finally, the theoretical results are compared with experimental measurements and a good agreement is observed.[1] R. Nava, V. Agarwal, J.A. del Río, C. Wang, *J. Non-Cryst. Solids* **329** (2003) 140.[2] L.T. Canham, *Appl. Phys. Lett.* **57** (1990) 1046.

Poster P-31

Title: A model of decagonal Al-Cu-Co based on a STEM image

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Abstract: Decagonal Al-Cu-Co had been modelled by Burkov [1], based on the electron microscopy [2] and x-ray diffraction data [3]. A variant of the model was latter founded over the decagonal tiling of the two golden triangles, $\mathcal{T}^{*(A_4)}$ [4], projected from the 4-dimensional root lattice A_4 . The recent STEM data of the same material [5] show that the previous models must be updated. We try to interpret the new data also as a decoration of the decagonal tiling $\mathcal{T}^{*(A_4)}$ and to construct the coding atomic surfaces.

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[5] S. Taniguchi, E. Abe, Highly-perfect decagonal quasicrystal $\text{Al}_{64}\text{Cu}_{22}\text{Co}_{14}$ with non-centrosymmetry, Phil. Mag. **88** (2008) 1949.

Poster P-32

Title: Nucleation and growth of a quasicrystalline bismuth monolayer on $i\text{-Al}_{70}\text{Pd}_{21}\text{Mn}_9$

Authors: J.A. SMERDON, •J.K. PARLE, L.H. WEARING

Address: Surface Science Research Centre and Department of Physics, The University of Liverpool, Liverpool L69 3BX, UK

Abstract: The formation of a Bi monolayer deposited on the five-fold surface of $i\text{-Al}_{70}\text{Pd}_{21}\text{Mn}_9$, has been studied by STM [1]. Upon deposition of low sub-monolayer coverage, the epitaxial growth of 5 atom pentagonal clusters of Bi atoms with edge length $4.9 \pm 0.3 \text{ \AA}$ is observed. The pentagons have a common orientation leading to a film with five-fold symmetry. By inspection of images where both the underlying surface and the Bi atoms are resolved, the pentagonal clusters are found to nucleate on pseudo-Mackay clusters truncated such that a Mn atom lies centrally in the surface plane. The initial nucleation site is different to that proposed on the basis of recent density functional theory calculations [2]. The Bi film grows in the pure nucleation regime (additional deposition results in the formation of new nuclei) until the saturation island density is reached at about half a monolayer. The density of these sites is sufficient to form a quasiperiodic framework. Above half a monolayer, the islands (pentagons) begin to coalesce, and the film growth enters a pure growth regime (adatoms will attach themselves with much higher probability to existing islands). This leads to the formation of a quasicrystalline monolayer. This work has recently been supported by XPS thermal desorption results [3], presented elsewhere at this conference, which show that the initial half monolayer has a higher binding energy than the rest of the monolayer. This explains the growth mode observed by STM (i.e. mainly higher binding energy nucleation sites are filled until saturated at $\sim 0.5\text{ML}$, then lower energy sites are filled until the monolayer is complete).

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Poster P-33**Title:** MEIS investigation of Fe thin film grown on *i*-Al₇₀Pd₂₁Mn₉**Authors:** J.A. SMERDON¹, J.K. PARLE¹, P. NUGENT¹, T. NOAKES², R. MCGRATH¹**Addresses:** ¹Surface Science Research Centre and Department of Physics, The University of Liverpool, Liverpool L69 3BX, UK ²CCLRC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK**Abstract:** The room temperature thin film growth of Fe deposited on the five-fold surface of *i*-Al₇₀Pd₂₁Mn₉ has been studied using Medium Energy Ion Scattering (MEIS). A complex growth mode is observed for Fe on this aperiodic quasicrystalline substrate. At coverages up to about 3 MLE (monolayer equivalent), layer-by-layer growth is observed whereby small clusters and islands are formed which eventually coalesce into almost complete monolayers. Previous Auger electron spectroscopy (AES) results show contradictory results, one study rules out intermixing [1], while another finds that Fe atoms do intermix with substrate [2]. The MEIS results clarify the question of intermixing. Above this coverage, there is a transition to a multilayer island growth mode. The islands have bcc(110) structure and are rotated by 72°, so the periodic Fe is related to the aperiodic substrate by 5-fold rotational epitaxy. MEIS is used to shed light on the structural composition of this transition region. The results are compared with previous work on Fe adsorption on this substrate using scanning tunneling microscopy (STM), low energy electron diffraction (LEED), and Auger electron spectroscopy (AES).[1] L.H. Wearing, J.A. Smerdon, L. Leung, T.A. Lograsso, A.R. Ross, R. McGrath, Surf. Sci. **601** (2007) 3450–3455.[2] Y. Weisskopf, R. Luscher, M. Erbudak, Surf. Sci. **578** (2005) 35.**Poster P-34**

see O-37

Poster P-35

see O-35

Poster P-36**Title:** A renormalization plus convolution approach to the electrical conductance of macroscopic aperiodic systems**Authors:** F. SANCHEZ, V. SANCHEZ**Address:** Departamento de Fisica, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico, Apartado Postal 70-542, 04510, D.F., Mexico**Abstract:** The electronic transport in macroscopic non-periodic lattices is an interesting but not widely addressed subject, since the transport of quantum particles and macroscopic aperiodic systems both per se are not easy topics. For example, there is a consensus that in quasiperiodic systems the electronic wave functions are critical and the corresponding eigenvalue spectra are singular continuous [1]. Hence, the transport properties of these critically localized states are a fascinating and still unclear theme. In this work, we report an extension of the renormalization plus convolution method to investigate the electrical conductivity of aperiodic lattice, such as Fibonacci systems [2], Thue-Morse and period-doubling ones [3]. This method combines the convolution theorem with the real-space renormalization technique, being able to address multidimensional aperiodic systems in a non-perturbative way. The results show a large number of transparent states with a unitary transmittance, contrary to the Fibonacci case. For two-dimensional systems, the conductance (g) spectrum shows a uniform stair structure for the periodic case and a fractal distribution of steps when the arrangement of atoms in the perpendicular direction becomes aperiodic. Moreover, the spectrally averaged conductance ($\langle g \rangle$) shows a power-law decay of $\langle g \rangle$ as the system length grows for both Fibonacci and period-doubling systems, and a beyond power-law behavior for the Thue-Morse case. For all these cases, $\langle g \rangle$ is neither constant as in periodic systems nor exponential decays occurred in randomly disordered lattices, revealing the peculiar localization nature in these aperiodic lattices. Finally, a comparative analysis of the ac conductance spectra obtained from the Kubo-Greenwood formula for these three aperiodic lattices will also be presented.

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Poster P-37**Title:** Escherlike quasiperiodic heterostructures**Authors:** A.G. BARRIUSO¹, J.J. MONZÓN¹, •L.L. SÁNCHEZ-SOTO¹, A.F. COSTA²**Addresses:** ¹Departamento de Optica, Facultad de Física, Universidad Complutense, 28040 Madrid, Spain ²Departamento de Matemáticas Fundamentales, Facultad de Ciencias, Universidad Nacional de Educación a Distancia, 28040 Madrid, Spain**Abstract:** Quasiperiodic heterostructures present unique structural, electronic, and vibrational properties, connected to the existence of incommensurate periods. We go beyond previous schemes, like Fibonacci or Thue-Morse, based on substitutional sequences, by introducing construction rules generated by tessellations of the unit disc by regular polygons. We explore some of the properties exhibited by these systems.**Poster P-38****Title:** Local atomic configurations of Al-Ni-Co decagonal clusters by first-principle calculations**Authors:** •T. SEKI¹, E. ABE¹, S.J. PENNYCOOK²**Addresses:** ¹Department of Materials Science & Engineering, The University of Tokyo, 113-8656, Japan ²Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA**Abstract:** Phason-related atomistic fluctuations cause several local configurations for the decagonal clusters that are the building-unit of decagonal quasicrystals. In the present work, we investigate the possible local configurations within the clusters of the approximant Al₇₁Ni₂₂Co₇ crystal, based on first-principle total energy calculations. The structure of approximant Al₇₁Ni₂₂Co₇ is represented as a periodic arrangement of fivefold symmetric decagonal clusters of 2nm across. We examine energy changes during switching local symmetry from fivefold to mirror, which can be achieved via phason-related localized atomistic behaviors.**Poster P-39****Title:** New type of aperiodic structure formed at first stages of crystallization of rare earth oxides and fluorides**Author:** I.M. SHMYTKO (PRESENTED BY V.F. DEGTYAREVA)**Address:** Institute of Solid State Physics, Chernogolovka, Moscow distr., 142432, Russia**Abstract:** Structure of nano-dispersed rare earth simple oxides Lu₂O₃, Gd₂O₃, Y₂O₃, La₂O₃ and Eu₂O₃, garnets Y₃Al₅O₁₂ and Y₃Ga₅O₁₂, perovskites YAIO₃ and LaAlO₃, borates LuBO₃, GdBO₃ and YBO₃, molybdate Eu₂(MoO₄)₃ and fluorides LuF₃ and Na₅Lu₉F₃₂ was investigated at first stages of crystallization. The oxides were received by high temperature annealing of amorphous precursor states. The amorphous precursor states were prepared by solvent thermolysis from a nitric-acid solution or an ammonium nitrate melt solution of simple oxides or nitrates of rare earth elements. LuF₃ was received by exchange reaction of water solution of lutetium nitrates with ammonium fluoride. Na₅Lu₉F₃₂ was prepared by solid phase synthesis from microcrystalline powders of LuF₃, NaF and ammonium fluoride.

X-ray investigations have shown that independently of synthesis method the first stages of crystallisation of such compounds are characterized by new structure state which can be characterized by set of isomorphous phases with continuous change of their lattice parameters. Infrared spectroscopy, Raman investigation and high resolution electron microscopy have shown that this state is realized in separate nano-grain and therefore can be declared as new type of aperiodic structure. The structure undergoes transformation into single phase with growth of nanocrystallites during consequent annealing.

The work was supported by RFBR no. 06-02-17298.

Poster P-40**Title:** The growth of C₆₀ on aperiodic and periodic allotropes of Cu**Authors:** •J.A. SMERDON¹, H.R. SHARMA¹, T.A. LOGRASSO², A.R. ROSS², R. MCGRATH¹**Addresses:** ¹Surface Science Research Centre and Department of Physics, The University of Liverpool, Liverpool, UK ²Ames Laboratory, Iowa State University, Ames, IA 50011, USA**Abstract:** Quasicrystals are extremely complex, both structurally and chemically [1]. The desire to study the complex geometry independently of the complex chemistry leads to the use of quasicrystals as templates for the growth of single-element quasicrystal films [2]. One such film is produced when Cu is grown using AlPdMn as a template. This film is composed of five orientational domains of material that is essentially crystalline, but with a small-scale superstructure modulation that manifests as a one-dimensional Fibonacci sequence in STM images from the film [3].

Carbon-60 is then used as a chemical probe to study the reactivity of this film. Although, in general, C₆₀ diffuses across Cu surfaces and forms islands with commensurate structures, this behavior is not observed on the aperiodically ordered Cu - rather, the C₆₀ molecules are so tightly bound that not only do they stick where they land, but internal cage structure may be observed by STM, indicating that the molecules cannot even rotate.

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[2] C. Francoual, F. Livet, M. de Boissieu, F. Yakhou, F. Bley, A. Letoublon, R. Caudron, J. Gastaldi, Phys. Rev. Lett. **91** (2003) 225501.

Poster P-42

Title: Synthesis of highly-ordered Zn-Fe-Sc quasicrystals and their physical properties

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Abstract: Zn-Fe-Sc quasicrystal is of a great interest since Fe atoms are reported to have a large magnetic moment. The magnetic susceptibility of the Zn-Fe-Sc quasicrystal follows the Curie-Weiss (CW) law with spin-glass like behavior at low temperatures ($T_f \approx 7.2\text{K}$) [1]. In addition, the Zn-Fe-Sc quasicrystal exhibits a unique temperature dependence of the electrical resistivity which has been discussed based on weak localization and Kondo effect [2]. In this paper, we will discuss the effect of the Fe concentration on the electrical resistivity as well as on the magnetic susceptibility of $\text{Zn}_{84-X}\text{Fe}_X\text{Sc}_{16}$ ($X=6.5-7.5$) prepared with high structural perfection. The magnetic susceptibility was observed to follow the CW law between 100 and 300K with a spin-glass like cusp at $T_f = 6.4\sim 7.2\text{K}$. When the Fe concentration is increased, T_f and Weiss temperature is found to increase linearly and the effective moment (μ_{eff}) was found to be nearly constant ($3.1 \sim 3.2\mu_B$), which implies that the exchange interaction in the Zn-Fe-Sc quasicrystals becomes more ferromagnetic with the increase of the Fe concentration. The correlation between the electrical resistivity and the Fe concentration will be discussed in detail.

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Poster P-43

Title: Orientational ordering of a tetrahedron in Cd- and Zn-based 1/1 approximants at low temperatures

Authors: •R. TAMURA¹, T. YAMADA¹, K. NISHIMOTO¹, Y. MURO², K. MOTOYA², C.P. GÓMEZ²

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Abstract: Low-temperature phase transitions of Cd- and Zn-based 1/1 approximants [1–3] are overviewed in terms of the superstructures formed as well as the entropy changes associated with the transitions. A similar type of ordering of a tetrahedron located at the cluster-center occurs for both Cd_6Ca and Zn_6Sc , which is characterized by a kind of an ‘antiferromagnetic order’, i.e., an antiparallel ordering of two orientations of the tetrahedron along the [110] direction of the high-temperature bcc phase. The transitions, on one hand, appear to be common behaviors of the approximants composed mainly of the group IIb elements. On the other hand, some variations have been noticed in the transition entropies, resulting in different number of states for the orientation of the tetrahedron above T_C , which will be compared with electron densities of the tetrahedron obtained from X-ray diffraction experiments above T_C . Detailed description of the differences in the transition behaviors between the compounds will be made and the transition phenomena will be discussed in terms of ordering of the tetrahedron at the center of the icosahedral cluster.

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Poster P-44**Title:** Similarity of eigenstates in generalized labyrinth tilings**Authors:** •S. THIEM, M. SCHREIBER**Address:** Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany**Abstract:** The eigenstates of d -dimensional quasicrystalline models with a separable Hamiltonian are studied within the tight-binding model. The approach is based on mathematical sequences, constructed by an inflation rule $\mathcal{P} = \{w \rightarrow s, s \rightarrow sws^{b-1}\}$ describing the weak/strong couplings of atoms in a quasiperiodic chain. Higher-dimensional quasiperiodic tilings are constructed as a direct product of these chains and their eigenstates can be directly calculated by multiplying the energies E or wave functions Ψ of the chain, respectively.

Applying this construction rule, the grid in d dimensions dissolves into 2^{d-1} different tilings, for which we investigated the characteristics of the wave functions. For the standard two-dimensional labyrinth tiling constructed from the octonacci sequence ($b = 2$) the lattice breaks up into two identical lattices, which consequently yield the same eigenstates. This is also true for the respective higher-dimensional systems, where 2^{d-1} identical lattices are found for $b = 2$ due to the palindromic structure. But for the corresponding generalized labyrinth tiling based on the Fibonacci sequence ($b = 1$) or for $b = 3$ this is not the case.

However, our numerical results show that also for $b \neq 2$ the wave functions of the different grids become increasingly similar for large system sizes. This can be explained by the fact that the structure of the 2^{d-1} grids only differs at the boundaries and thus for large systems the eigenstates approach each other. This property allows us to analytically derive properties of the higher-dimensional generalized labyrinth tilings from the one-dimensional results. In particular participation numbers and corresponding scaling exponents have been determined.

Poster P-45**Title:** Stability of nano-crystalline τ_3 phases during vacuum and air annealing**Authors:** •T.P. YADAV¹, N.K. MUKHOPADHYAY², R.S. TIWARI¹, O.N. SRIVASTAVA¹**Addresses:** ¹Department of Physics, Banaras Hindu University, Varanasi 221005, India²Department of Metallurgical Engineering, Institute of Technology, Banaras Hindu University, Varanasi 221005, India**Abstract:** A nano τ_3 vacancy-ordered phase in the Al-Ni-Cu alloy system has been synthesized with a composition close to $\text{Al}_{70}\text{Cu}_{15}\text{Ni}_{15}$ by mechanical alloying of a mixture of elemental powder in a high-energy ball mill by varying milling time from 10 to 100 hours under liquid hexane medium. The stability of nano-crystalline τ_3 vacancy-ordered phases has been studied under thermal annealing in vacuum as well as in air. The X-ray diffraction and transmission electron microscopy techniques were employed for characterization of the milled and annealed samples. The powder after 100 h of milling was found to contain mostly nano τ_3 phases with the partial ordering, and with crystallite sizes in the range 10–20 nm along with a lattice strain of $\sim 0.67\%$. The milled powder, after annealing in vacuum at 700 °C 60 h, revealed the formation of a strain-free and ordered τ_3 phase with a crystallite size of 80 nm, indicating grain coarsening. It is interesting to note that the milled powder annealed in air at 700 °C for 60 h showed the formation of $(\text{Cu,Ni})\text{Al}_2\text{O}_4$ type spinel phase with the lattice parameter of 8.1 Å and the lattice strain as 0.52 %. The average grain size of spinel phase was found to be ~ 40 nm. The photoluminescence and UV-Visible spectrometer was used for optical properties measurements. The evolution of nanostructured phases and their stability was discussed with respect to their optical properties.

Poster P-46**Title:** Characterisation of Bi growth on the Quasicrystal *i*-AlPdMn**Authors:** J.A. SMERDON, V. DHANAK, •K. YOUNG, N. CROSS, H.R. SHARMA, R. MCGRATH**Address:** Surface Science Research Centre and Department of Physics, The University of Liverpool, Liverpool L69 3BX, UK**Abstract:** Bismuth was one of the first elements that was shown to form a quasicrystalline layer when deposited on quasicrystalline substrates [1]. The Bi/AlPdMn system is a rich one and has been extensively studied using STM, LEED and HAS [1–3]. We present results from XPS that further illuminate the growth of this system, in particular establishing the growth as a version of the Stranski-Krastanov mode. The fivefold LEED pattern obtained from the monolayer of Bi is similar to that from the clean surface, indicating pseudomorphic growth.

Desorption curves have been obtained by directly heating the sample and subsequently collecting XPS data. The curves are highly consistent with all previous data [1,2], showing peaks in thermodynamic stability of the layer at around 1 ML and 0.4 ML coverage. This indicates that a large number of Bi atoms are situated in significantly energetically favourable sites on the quasicrystal surface, supporting the nucleation hypothesis presented in reference [2].

Finally, an interesting experiment conducted some days after the initial work has indicated that the Bi layer passivates the surface against oxygen contamination under UHV. This passivation, however, does not hold for exposure to atmospheric conditions.

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[3] H.R. Sharma, M. Shimoda, A.P. Tsai, Advances in Physics **56** (2007) 403–464.**Poster P-47****Title:** Multiplicativity in the theory of coincidence site lattices**Author:** P. ZEINER**Address:** Faculty of Mathematics, Bielefeld University, Bielefeld, Germany**Abstract:** Coincidence Site Lattices (CSLs) are a well established tool in the theory of grain boundaries. For several lattices up to dimension $d = 4$, the CSLs are known explicitly as well as their indices and multiplicity functions. Many of them share a particular property: their multiplicity functions are multiplicative. We show how multiplicativity is connected to certain decompositions of CSLs and the corresponding coincidence rotations and present some criteria for multiplicativity. In general, however, multiplicativity is violated, while supermultiplicity still holds.

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