

Program of Oral Presentations

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Monday, June 14, 2010

Session 1: Formation (chair: A.P. Tsai)

8:40-9:20 S01-01*	P.C. Canfield, M.L. Caudle, C.-S. Ho, A. Kreyssig, S. Nandi, M.G. Kim, X. Lin, A. Kracher, K.W. Dennis, R.W. McCallum and <u>A.I. Goldman*</u> i-Sc ₁₂ Zn ₈₈ : A new binary icosahedral quasicrystal
9:20-9:40 S01-02	M. de Boissieu, T. Yamada, C. Cui, H. Euchner, C. Pay Gomez and A.P. Tsai Structural quality, diffuse scattering and phasons modes in the AgInYb icosahedral phase
9:40-10:00 S01-03	W. Steurer Factors governing growth and stability of quasicrystals and other complex intermetallics
10:00-10:20 S01-04	U. Mizutani and H. Sato Hume-Rothery stabilization mechanism and d-states-mediated-Fermi surface-Brillouin zone interactions in structurally complex metallic alloys

Session 2: Formation and Structures (chair: W. Steurer)

10:40-11:20 S02-01*	M. Engel*, A. Haji-Akbari, E.R. Chen and S.C. Glotzer Quasicrystalline phase of densely packed tetrahedron
11:20-12:00 S02-02*	C. Xiao, K. Miyasaka, N. Fujita, Y. Sakamoto and <u>O. Terasaki*</u> Dodecagonal tiling in mesoporous silica

Session 3: New systems (chair: R. Lifshitz)

13:30-14:10 S03-01*	T. Dotera* Structural transition of dodecagonal quasicrystals and approximants
14:10-14:50 S03-02*	C. Bechinger*, J. Mikhael, L. Helden and T. Bohlein Colloidal monolayers on quasiperiodic light fields

Session 4: Structures (chair: P. Thiel)

15:10-15:50 S04-01*	H. Takakura* Structural feature of Yb-Cd type icosahedral quasicrystal
15:50-16:10 S04-02	M. Mihalkovič, M. Krajčič, C.L. Henley and J. Hafner Low-temperature structure of i-AlMnPd approximants from energetic optimization: covering by "Pseudo-Mackay" clusters
16:10-16:30 S04-03	H. Orsini-Rosenberg and W. Steurer <i>Ab initio</i> investigations on the stability of sevenfold approximants
16:30-16:50 S04-04	A. Yamamoto Short-range order diffuse scattering intensity in d-Al-Ni-Co s1 and b-Ni phases

Tuesday, June 15, 2010

Session 5: Physical properties (chair: J. Dolinšek)

8:40-9:20 S05-01*	A. Smontara* Anisotropic transport properties of complex metallic alloys
9:20-9:40 S05-02	M.A. Chernikov and Yu.Kh. Vekilov Fermi-surface effects in icosahedral quasicrystals
9:40-10:00 S05-03	J.-M. Dubois and E. Belin-Ferré Electronic properties versus lattice complexity in Al-based complex metallic alloys
10:00-10:20 S05-04	S.E.-D. Mandel and R. Lifshitz The Fibonacci quasicrystal - new surprises from an old model

Tuesday, June 15, 2010

Session 6: Physical properties (chair: J. Wolny)

10:40-11:00 S06-01	<u>A. Jagannathan</u> and E.Y. Vedmedenko Quasiperiodic antiferromagnet with pentagonal loops
11:00-11:20 S06-02	<u>R. Tamura</u> , Y. Muro, T. Hiroto, H. Yaguchi and T. Takabatake Magnetic properties of Cd ₆ R 1/1 approximants
11:20-11:40 S06-03	<u>T. Watanuki</u> , D. Kawana, A. Machida and A.P. Tsai Valence fluctuation state in Yb based quasicrystals
11:40-12:00 S06-04	<u>H. Euchner</u> , M. Mihalkovič, M.R. Johnson, H. Schober, A.P. Tsai, S. Ohhashi, C. Gomez, S. Lidin and M. de Boissieu Lattice dynamics in complex zinc-magnesium phases

Session 7: Surfaces (chair: V. Fournée)

13:30-14:10 S07-01*	<u>H.R. Sharma*</u> , P.J. Nugent, G. Simutis, J. Smerdon, V.R. Dhanak, R. McGrath, M. Shimoda, C. Cui, Y. Ishii and A. P. Tsai Surfaces of icosahedral Cd-Yb family quasicrystal: structure, electronic properties and epitaxy
14:10-14:30 S07-02	C. Yuen, B. Ünal, D. Jing and <u>P.A. Thiel</u> Surface segregation in an Al-based quasicrystal: Zn in decagonal Al-Pd-Zn
14:30-14:50 S07-03	R. Addou, A. Shukla, M.-C. de Weerd, P. Gille, R. Widmer, V. Fournée, O. Gröning, J.-M. Dubois and <u>J. Ledieu</u> Cu adsorption on the (100) surface of the Al ₁₃ Co ₄ approximant
14:50-15:10 S07-04	<u>M. Krajčí</u> and J. Hafner Catalytic properties of Al ₁₃ Co ₄ studied by <i>ab initio</i> methods

Session 8: Mathematics (chair: M. Baake)

15:30-16:10 S08-01*	<u>F. Gähler*</u> Topological invariants of aperiodic tilings
16:10-16:30 S08-02	<u>J.-Y. Lee</u> and S. Akiyama Determining quasicrystal structure on substitution tilings
16:30-16:50 S08-03	<u>P. Zeiner</u> and M. Loquias Colourings of lattices and CSLs

Wednesday, June 16, 2010

Session 9: Mathematics (chair: S. Ben-Abraham)

8:40-9:00 S09-01	<u>M.L.A.N. De Las Peñas</u> , E.P. Bugari and D. Frettlöh Colourings of cyclotomic integers with class number one
9:00-9:20 S09-02	<u>N. Fujita</u> Point substitution processes for generating icosahedral tilings
9:20-9:40 S09-03	<u>M. Baake</u> and H. Kösters Random point sets and their diffraction

Session 10: Dr. Stefan Ritsch Memorial (chair: R. Lück)

10:00-10:05	<u>R. Lück</u>
10:05-10:25 S10-01	<u>P. Kuczera</u> , J. Wolny and W. Steurer The structure of decagonal Al-Ni-Co superstructure type I
10:25-10:45 S10-02	<u>A. Strutz</u> , A. Yamamoto and W. Steurer Superstructure determination of basic Co-rich decagonal Al-Co-Ni
10:45-11:05 S10-03	<u>E. Abe</u> , T. Seki and S.J. Pennycook Point-defect distributions in an ideal Al ₇₂ Ni ₂₀ Co ₈ studied by ultrahigh-resolution STEM and first-principle calculations

Thursday, June 17, 2010

Session 11: Physical properties (chair: M. Chernikov)

8:40-9:00 S11-01	R. Mäder, R. Widmer, P. Ruffieux and O. Gröning Correlating the local density of states and the macroscopic conductivity in quasicrystals and approximants
9:00-9:20 S11-02	G. Trambly de Laissardière, C. Oguey, and D. Mayou Metal insulator transition induced by long range quasiperiodic order in octagonal tiling
9:20-9:40 S11-03	V.R. Misko, D. Bothner, M. Kemmler, R. Kleiner, D. Koelle, F.M. Peeters, and F. Nori Enhancing the critical current in superconductors with quasiperiodic pinning arrays below and above the matching flux
9:40-10:00 S11-04	F. Rösch and H.-R. Trebin Brittle fracture of a complex metallic compound from an atomistic viewpoint

Session 12: Applications (chair: R. McGrath)

10:20-10:40 S12-01	H. Somekawa, A. Singh, Y. Osawa and T. Mukai Mg-Zn-Al alloys containing quasicrystal and related phases for structural applications
10:40-11:00 S12-02	X. Wang, Z. Zhang and L. Wang Preparation and wear resistance of Ti-Zr-Ni quasicrystal and polyimide composite materials
11:00-11:20 S12-03	S. Kenzari, D. Bonina, J.-M. Dubois and V. Fournée Selective laser sintering of quasicrystalline preforms: A new technological application for manufacturing functional Al-based parts
11:20-11:40 S12-04	K. Biswas, S. Kameoka, Y. Xu and A.P. Tsai A novel catalyst fabricated from Al-Co-Ni decagonal quasicrystal for steam reforming of methane
11:40-12:00 S12-05	V.K. Vani, S.M. Hong and E. Fleury Synthesis of porous Cu thin films from RF sputtered quasicrystalline Al-Cu-Co alloy thin films

Session 13: Applications (chair: K. Kimura)

13:30-13:50 S13-01	T. Takeuchi, H. Goto and M. Mikami Development of thermal rectifier using the unusual electron thermal conductivity of quasicrystals
13:50-14:10 S13-02	J. Dolinšek, M. Jagodič, Z. Jagličić, M. Feuerbacher and M. Heggen Thermal storage of digital information in the Taylor-phase decagonal approximants
14:10-14:50 S13-03*	X. Zhang* Negative refraction and localized states of classical wave in high-symmetry quasicrystals

Session 14: Related topics (chair: M. de Boissieu)

15:10-15:50 S14-01*	S. Lee*, R. Berger and R. Hoffmann Gamma-brass superstructures, perpendicular pseudo-5-fold axes, and the E8 lattice
15:50-16:30 S14-02*	S. van Smaalen* Modulated structures of low-dimensional electronic and magnetic crystals
16:30-16:50 S14-03	K. Kimura, H. Hyodo, Y. Takagiwa, K. Kirihaara, K. Soga, K. Kato and M. Takata Self-compensation and bonding-conversion in B-based and Al-based icosahedral cluster solids

Friday, June 16, 2010

Session 15: Formation and New system (chair: C. L. Henley)

8:40-9:20 S15-01*	<u>P.J. Steinhardt*</u> Once upon a time in Kamchatka: the search for natural quasicrystals
9:20-10:00 S15-02*	<u>Y. Matsushita*</u> Kaleidoscopic structures with mesoscopic length scales from ABC terpolymer systems

Closing (chair: T. Ishimasa)

10:10-10:40	<u>J.-M. Dubois and R. Lifshitz</u> Concluding Remarks
10:40-10:55	Young Scientist Award
10:55	Announcement of ICQ12

Oral Presentations

i-Sc₁₂Zn₈₈: A new binary icosahedral quasicrystal

P. C. Canfield,^{1,2} M. L. Caudle,² C.-S. Ho,¹ A. Kreyssig,^{1,2} S. Nandi,^{1,2} M. G. Kim,^{1,2} X. Lin,^{1,2} A. Kracher,¹ K. W. Dennis,¹ R. W. McCallum,^{1,3} and A. I. Goldman^{1,2}

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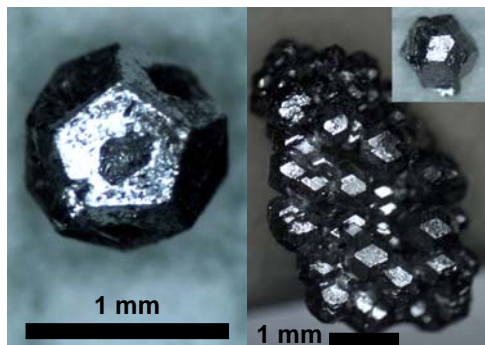
³*Department of Materials Science and Engineering, Iowa State University, Ames, Iowa 50011, USA*

Although they form, almost readily, in a wide variety of ternary and quaternary metallic alloys, examples of stable binary icosahedral quasicrystals are quite rare. Indeed, it has been a decade since the discovery of icosahedral phases in Cd-Yb and Cd-Ca.[1,2] The Sc-Zn system has been associated with quasicrystal formation for some time. An icosahedral phase has been identified in Sc₁₅Mg₅Zn₈₀ [3] and a large number of ternary and quaternary compositions of the type Sc-*M*-Zn (*M*=Mn, Fe, Co, Ni, Cu, Pd, Pt, Au, and Ag). In addition, the binary crystalline alloy ScZn₆ has been identified as an approximant of the icosahedral phase. Despite all of this study, the binary “parent” icosahedral phase in the Sc-Zn system has eluded detection. As part of the exploration of the Sc-Zn binary phase diagram using flux-growth, we have discovered millimeter-sized faceted grains of i-Sc₁₂Zn₈₈ with icosahedral (pentagonal dodecahedral and rhombic triacontahedral) morphologies. Structural characterization of the icosahedral phase was accomplished through conventional x-ray powder diffraction measurements and single grain high-energy x-ray diffraction which enables large regions of reciprocal space to be probed. For both growth morphologies all diffraction peaks could be indexed by a primitive (*P*-type) icosahedral phase pattern according to the icosahedral group *m*35 with a quasilattice constant of 5.017(3) Å. The two types of morphology do, however, present interesting differences in their respective degrees of quasicrystalline order. We have also annealed as-grown samples at 390 °C for 22 h in one atmosphere of Ar and found neither morphological nor structural changes as evidenced by visual inspection, the x-ray Laue pattern, and x-ray powder diffraction, further indicating that the icosahedral phase is stable.

[1] A. P. Tsai, J. Q. Guo, E. Abe, H. Takakura, and T. J. Sato, *Nature (London)* **408**, 537 (2000).

[2] J. Q. Guo, E. Abe, and A. P. Tsai, *Phys. Rev. B* **62**, R14605 (2000).

[3] Y. Kaneko, Y. Arichika, and T. Ishimasa, *Philos. Mag. Lett.* **81**, 777 (2001).



Facetted morphologies of i-Sc₁₂Zn₈₈ found in flux-grown samples

STRUCTURAL QUALITY, DIFFUSE SCATTERING AND PHASONS MODES IN THE AgInYb ICOSAHEDRAL PHASE

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Recently, it has been shown that centimeter size single grains of the icosahedral phase can be grown in the Ag-In-Yb system [1]. The icosahedral phase is believed to be isostructural to the i-CdYb icosahedral phase [2], the Cd being replaced by a Ag-In mixture. We present results on the study of the structural quality and diffuse scattering of the AgInYb icosahedral quasicrystal, obtained using high resolution x-ray scattering on the D2AM beam line of the ESRF. Systematic Q-scans along the high symmetry axes could be indexed with a primitive icosahedral lattice. The maximum Q_{perp} value necessary for indexing the diffraction pattern has been found to be equal to 5 (r.l.u.) i.e. smaller than for ZnMgSc quasicrystals [3]. The crystal quality has been found to be extremely good, with rocking curves having FWHM width equal to 0.01° and with a small Q_{perp} dependence of the width which has been found to be linear. The slope is equal to 5×10^{-4} , i.e. similar to the best known quasicrystal so far [4] and indicates a small residual phason strain distribution in the sample.

Systematic reciprocal space maps display a clear distribution of diffuse scattering around the Bragg reflections. As for other quasicrystals [5] the diffuse scattering can be interpreted as resulting mainly from long wavelength phason modes. However the shape anisotropy of the diffuse scattering points towards a positive ratio of the K_2/K_1 phason elastic constants, related to 5-fold rather than 3-fold instabilities. Those results will be compared to the one obtained for the CdYb phase. Implications of those findings for atomistic modeling of long wavelength phason modes will also be discussed.

1 . Cui C and Tsai A P 2010 J of Crystal Growth **312** 131.

2 . Takakura H, Gomez C P, Yamamoto A, de Boissieu M and Tsai A P 2007 Nature Materials **6** 58.

3 . de Boissieu M, Francoual S, Kaneko Y and Ishimasa T 2005 Phys. Rev. Lett. **95** 105503.

4 . Letoublon A, Yakhou F, Livet F, Bley F, de Boissieu M, Mancini L, Caudron R, Vettier C and Gastaldi J 2001 Europhysics Letters **54** 753.

5 . Janssen T, Chapuis G and de Boissieu M, *Aperiodic Crystals. From modulated phases to quasicrystals* 466 pages (Oxford University Press, Oxford, 2007)

FACTORS GOVERNING GROWTH AND STABILITY OF QUASICRYSTALS AND OTHER COMPLEX INTERMETALLICS

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Already the early rapid solidification experiments on Al-Mn have shown that quasicrystals (QC) can grow much faster than their approximants. This has been mainly attributed to the lower nucleation barrier of QC due to the local icosahedral order already present in the melt. This does not explain, however, how quasiperiodic long-range order is established without much diffusion and why never high rational approximants are formed instead. What lets quasiperiodic order win over the periodic order of approximants? The fundamental clusters are in both cases equally distorted, they are far from ideal icosahedral symmetry. Why are quasiperiodic structures closer to ideal quasiperiodicity than to the averaged one of random tilings?

We will present models that offer answers to these questions. Beside other factors, particularly the role of flat atomic layers for the growth and stability of QC and other complex intermetallics will be discussed. An example is illustrated in Fig. 1, where the projected structures of an icosahedral QC, its 1/1-approximant and the largest known intermetallic structure are shown. All atoms of the QC are located on sets of flat atomic layers which obey the icosahedral symmetry. A completely different picture is obtained along the pseudo-5-fold direction of the 1/1-approximant although the local structures are similar. It is also remarkable that all structures of large periodic intermetallics show an analogue abundance of flat atomic layers what is already well known for Frank-Kasper phases.

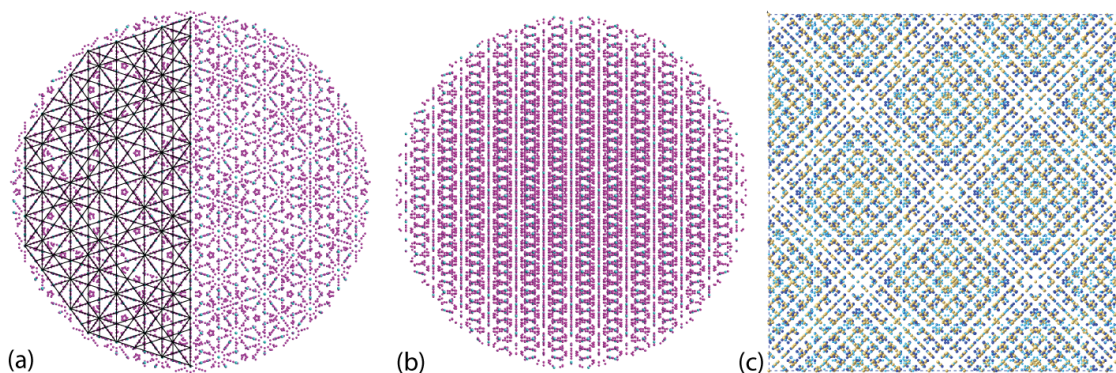


Fig. 1 Projections of the structures of (a) $i\text{-Cd}_{84}\text{Yb}_{16}$ along the 5-fold axis, (b) $1/1\text{-Cd}_6\text{Yb}$ along the pseudo-5-fold axis and (c) $cF(23,256-x)\text{-Al}_{55.4}\text{Cu}_{5.4}\text{Ta}_{39.1}$ along $[100]$.

**HUME-ROTHERY STABILIZATION MECHANISM AND
d-STATES-MEDIATED-FERMI SURFACE-BRILLOUIN ZONE
INTERACTIONS IN STRUCTURALLY COMPLEX METALLIC ALLOYS**

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There are two mechanisms for the formation of a pseudogap across the Fermi level in complex metallic alloys (CMAs): one the Fermi surface-Brillouin zone (FsBz) interactions and the other orbital hybridizations. It is important to remind that the FsBz interactions are applied only to crystals and quasicrystals, where diffraction spectrum consists of a series of δ -functions, and, hence, are structure- and e/a -sensitive. On the other hand, the orbital hybridizations can occur not only in crystals but also in amorphous alloys and even in liquids, where the Bragg peaks are lost. Hence, the structure- and e/a -dependent phase stability can be pursued only through the FsBz interactions. We consider the frequently cited phrase "Hume-Rothery stabilization mechanism" to be designated only to the situation, where the phase stabilization can be discussed in terms of the FsBz interactions. However, the phrase "Hume-Rothery stabilization mechanism" has been frequently employed upon discussing the Hume-Rothery electron concentration rule for quasicrystals characterized by an orbital hybridization-induced pseudogap. We have recently introduced the concept of "d-states-mediated FsBz interactions" [1], which is capable of explaining the e/a - and structure-dependent phase stability even for strongly orbital-hybridizing systems.

Discussions will be focused on three themes:

1. The phase stability for the $\text{Co}_2\text{Zn}_{11}$, Al_8V_5 gamma-brasses and Al-Cu-TM (TM=Fe and Ru) 1/1-1/1-1/1 approximants will be systematically interpreted in terms of d-states mediated FsBz interactions.
2. The formation mechanism of a pseudogap in the RT-type Al-Mg-Zn 1/1-1/1-1/1 approximant will be presented.
3. The stability range of gamma-brasses, 1/1-1/1-1/1 approximants, including RT-, MI- and Tsai-type ones, and 2/1-2/1-2/1 approximants can be decisively specified by the number of electrons per unit cell, e/uc , provided that the e/a value is reliably determined by the *Hume-Rothery* plot we developed on the basis of the first-principles FLAPW band calculations. This is taken as the evidence for the validity of the FsBz or d-states mediated FsBz interactions or the Hume-Rothery stabilization mechanism for all CMAs characterized by a pseudogap at the Fermi level.

[1] U.Mizutani, "*Hume-Rothery Rules for Structurally Complex Alloy Phases*" (Taylor & Francis, 2010)

Quasicrystalline Phase of Densely Packed Tetrahedra

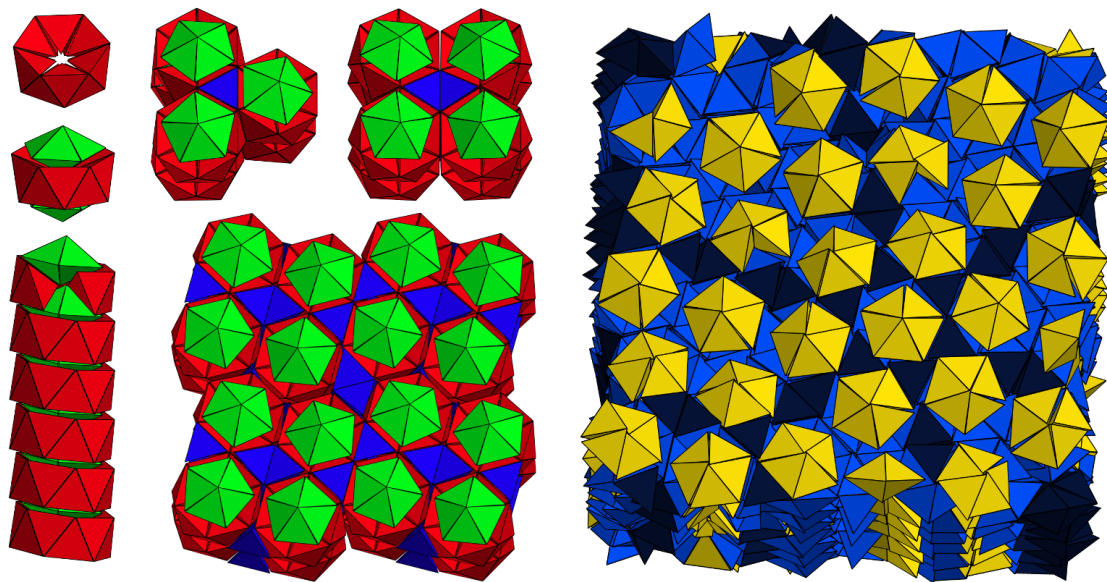
M. Engel¹, A. Haji-Akbari¹, E.R. Chen², and S.C. Glotzer^{1,3}

¹*Department of Chemical Engineering*, ²*Department of Mathematics*, ³*Department of Materials Science and Engineering, University of Michigan, Ann Arbor Michigan 48109, USA*

Although quasicrystals are traditionally found in alloys, there is increasing experimental evidence that they might be more common than previously thought. Here we report the observation of spontaneous ordering in a system of hard, anisotropic particles. Using Monte Carlo simulations, we observe that a fluid of hard tetrahedra undergoes a first-order transition to a dodecagonal quasicrystal. Its structure is characterized as a complex network of pentagonal dipyramids and tetrahelices. By compressing an approximant, the highest observed packing fraction is 85.03% – much higher than previously reported tetrahedron packing densities. Furthermore, we present the currently densest known packing of regular tetrahedra with density 85.63% and discuss its relative stability compared to the quasicrystal.

[1] A. Haji-Akbari, M. Engel et al., *Nature* 462, 773 (2009)

[2] E.R. Chen, M. Engel and S.C. Glotzer, arXiv:1001.0586



DODECAGONAL TILING IN MESOPOROUS SILICA

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and Osamu Terasaki^[1,2]

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A mesoporous silica crystal is formed through co-operative self-organisation of surfactant and silica precursor in silica-surfactant-water system. We have succeeded in synthesising a mesoporous silica crystal, which indicates twelve-fold symmetry in both morphology and electron diffraction pattern as shown in Figures 1 and 2, respectively. A transmission electron microscope image from a section of the crystal shows an aperiodic tiling in the central part, which is surrounded by twelve fans with more periodic tilings. The 2d tiling and 3d structure correlation has been established from the understanding of the relevant 3d-structures of mesoporous silica crystals with space groups of $Pm\bar{3}n$, $P4_2/mnm$ and newly determined $Cmmm$. The central tiling is carefully analysed in terms of phason strain based on dodecagonal quasiperiodic tiling. This indicates great promise to obtain a quasiperiodic tiling with 12-fold symmetry in mesoporous silicas by tuning the synthesis condition. The relationship between the lattice type and the growth mechanism will be also discussed based on the results.

The morphology of the mesoporous silica crystal (Figure 1) and the electron diffraction pattern from the central part of the sectioned crystal (Figure 2)

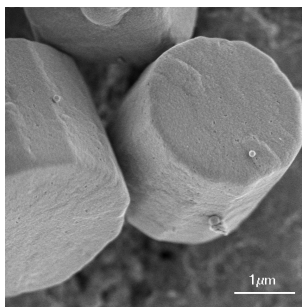


Figure 1

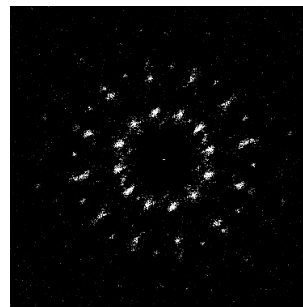


Figure 2

STRUCTURAL TRANSITION OF DODECAGONAL QUASICRYSTALS AND APPROXIMANTS

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Dodecagonal quasicrystals and related approximants (Archimedean tilings) cover a wide variety of materials, demonstrating that the dodecagonal order is universal over different length-scales: The edge lengths of polygons are ~ 0.5 nm for metallic alloys, ~ 2 nm for chalcogenide, ~ 10 nm for liquid crystalline organic dendrons, ~ 20 nm for binary nanoparticles, and ~ 50 nm for ABC star terpolymers¹. Furthermore, it has been numerically shown that complex potential systems, a lattice polymeric alloy system², and a tetrahedral packing system show dodecagonal order without any input of dodecagonal symmetry. Even if the physical origin of these formations differs, all structures consist of common structural units, squares and equilateral triangles.

In this contribution, we present a simulation study of structural transformation of square-triangle tilings in terms of “defect-mediated” phason flips. In contrast to a zipper rearrangement of squares and triangles^{3,4}, which sometimes becomes a wide-area rearrangement, defect-mediated phason flips enable us to update tiling locally with recourse to the inclusion of other polygons, i.e. skinny rhombi, hexagons and heptagons, which has been observed in TEM images of dodecagonal alloys. We move vertices with physically acceptable restrictions in order to prevent the tiling from being broken into pieces. Since the update move is local, the Metropolis Monte Carlo algorithm including the evaluation of energy differences, can be easily implemented.

Using the new algorithm, we have found that depending on local energies, the tiling system transforms into different low temperature phases: two-phase separations into 4^4 and 3^6 tilings, multiple twins of 3^34^2 tilings, or mixture phases of several approximants of dodecagonal quasicrystals. We will compare the simulation results with polymer and related experiments.

[1] K. Hayashida, et. al., Phys. Rev. Lett. **98** (2007) 195502.

[2] T. Dotera, Phil. Mag. **88** (2008) 2245.

[3] M. Oxborrow and C. L. Henley, Phys. Rev. B **48** (1993) 6966.

[4] J. Roth, Z. Kristallogr. **223** (2008) 761.

COLLOIDAL MONOLAYERS ON QUASIPERIODIC LIGHT FIELDS

C. Bechinger, J. Mikhael, L. Helden, T. Bohlein

2. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

Monolayers of interacting colloidal particles have been established as versatile model systems to address fundamental questions in the context of structural and dynamical processes in atomic systems. Due to their mesoscopic length and time scale, the trajectories of individual colloidal particles can be conveniently traced with optical methods. In addition, such systems respond very sensitive to external forces such as optical fields. This allows creating quasiperiodic potential landscapes with different rotational symmetries by means of interfering laser beams. In this talk we demonstrate, how colloidal monolayers can be used to study fundamental questions regarding the phase behavior, the growth and the friction of thin layers deposited on quasicrystalline surfaces.

**STRUCTURAL FEATURE OF Yb-Cd TYPE ICOSAHEDRAL
QUASICRYSTALS**

Hiroyuki Takakura

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Icosahedral quasicrystals of the Yb-Cd type form a large family among quasicrystals. Most of the known stable icosahedral phases in this category are ternary alloys. Therefore, it is an intriguing question that which constituent elements occupy where in the structures, since such structural information is essential for a better understanding of atomic interaction in quasicrystals. The structural description with rhombic triacontahedron (RTH) clusters enables us to compare the approximant crystals and quasicrystals in this system in a unified way. In this talk I will review the characteristic features of the Yb-Cd type icosahedral quasicrystals as aggregations of the RTH clusters. Further I will discuss chemical order in the quasicrystals from the point of view of geometrical constraints with help from recently refined ternary structures.

**LOW-TEMPERATURE STRUCTURE OF *i*-AlMnPd
APPROXIMANTS FROM ENERGETIC OPTIMIZATION:
COVERING BY “PSEUDO-MACKAY” CLUSTERS**

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i-AlMnPd is perhaps the best established and most studied stable quasicrystal. Yet, none of the models described to date [1] achieves a reasonable total energy, as compared to the tie-plane of the competing crystalline phases, namely the ternary phases “*T*” or ξ -AlMnPd, and the binary Al₃Pd₂. Our extensive optimization effort combines realistic fitted pair potentials and first-principle total energy calculations, with molecular dynamics and lattice gas annealing methods, to discover low-temperature optimal structures. We find that in the optimal structure of *i*-AlMnPd approximants, $\sim 90\%$ of the volume is accounted by chemically ordered pseudo-MI (pMI) clusters, whose icosahedrally symmetric second shell (Mn/Pd-icosahedron and Al-icosidodecahedron) encapsulates a low-symmetric inner shell composed of one Mn atom surrounded by 10 Al atoms. The clusters form a network with linkages along the 2-fold and 3-fold axes; taking the filling of the spaces between clusters, the whole structure is well described as a “canonical cell” tiling [2], with pMI on the even vertices, and (single-shell) Pd-centred Al₁₂ icosahedra on the odd vertices. The orientation of each inner-shell Al cluster is constrained by the arrangement of other pMI clusters in its neighborhood.

For comparison to the six-dimensional-cut representation of quasicrystal structures [1], we note that all atoms except the inner Al shell of pMI lie close to ideal atomic positions projected from 6D space. In contrast, the inner-shell Al atoms are often as far as 1 Å away from the ideal sites. Thus according to our findings, $\sim 78\%$ of the atoms in *i*-AlMnPd are “framework” atoms on 6D-projected sites, whereas 22% of the atoms belong to the highly variable 10-atom inner-shell clusters.

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***AB INITIO* INVESTIGATIONS ON THE STABILITY OF
SEVENFOLD APPROXIMANTS**

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Sevenfold symmetry is the lowest rotational symmetry not yet observed in quasicrystals. However, there are several strong hints that indicate the existence of heptagonal quasicrystals [1]. In rare earth transition metal borides and borocarbides, several layered structure types can be understood as approximants of two-dimensional sevenfold quasicrystals. 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, YCrB₄ (consisting of the "fat" and "thin" rhomb) and ThB₄ ("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.

The first-principles DFT calculations were performed with the VASP code [2], using a plane-wave basis set, the GGA algorithm and PAW-PBE pseudopotentials. Total energies of the approximant structures were calculated in five different ternary systems, B-Cr-RE (RE = Dy, Er, Ho, Y) and B-Mn-Dy. Additionally, decagonal boron-based layered approximants, that are not chemically stable in the respective ternary systems, were constructed from known stable structure types by chemical substitution (*e.g.* ReY₃B₇-type, ThMoB₄-type, ...). This was done to be able to compare the stability of local decagonal ordering with heptagonal ordering. Relaxation calculations were performed on all theoretical approximants to confirm their mechanical stability. Convex hulls for the ternary systems were constructed from the total energies of all theoretical approximants, as well as all stable ternary and binary structures known in these systems. From our results we will conclude which systems are most stable and suitable for future experimental research towards sevenfold quasicrystals.

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SHORT-RANGE ORDER DIFFUSE SCATTERING INTENSITY IN D-AL-NI-CO S1 AND B-NI PHASES

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There are several decagonal phases in Al-Ni-Co alloys. Among them, the S1 and b-Ni phases are the low and high temperature phases of d-Al₇₁Ni₁₈Co₁₁. They are both considered to be composed of the 20Å clusters but with different symmetry. The clusters in both phases are located at the vertices of the pentagon Penrose pattern with an edge length of about 20Å. In the former the cluster has 5-fold symmetry, while the latter has only a mirror.[6] Recently a diffuse scattering intensity formula in quasicrystals is proposed.[4, 5] In this paper, we apply it to these two phases to demonstrate the efficiency of the formula in the analysis of disordering in quasicrystals. It is known that in d-Al-Ni-Co the correlation length of atoms is not really of short range and medium range order correlation ranging up to several tens Å exists[1, 2, 3]. When we consider the orientational disordering of the clusters, we can easily include such a medium range order correlation in the analysis. We consider the correlation of the clusters up to the third nearest cluster neighbor. The inter-cluster distances for the first, second and third nearest neighbors are about 12, 20 and 32Å respectively. According to the models of the ideal S1 and b-Ni phases, the correlation between these clusters up to these neighbors in the ideal quasicrystals structure can be calculated. For a real structure at around the transition temperature between these phases, we may consider the correlation up to 32Å which is the same as in the ideal structures and may neglect the correlation longer than these inter-cluster distances as the first approximation. The diffuse scattering intensity of the S1-phase in the zero-th approximation, in which the inter-cluster correlation is neglected, is given by Kobas et al.[3]. The effect of the inter-cluster correlation in the diffuse scattering intensity will be discussed.

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Anisotropic Transport Properties of Complex Metallic Alloys

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Anisotropic transport properties (electrical resistivity, thermoelectric power, and thermal conductivity) of the o -Al₁₃Co₄, Al₁₃Fe₄, and T-Al_{72.5}Mn_{21.5}Fe₆ complex metallic alloys from the Al₁₃TM₄ intermetallic system were investigated. The investigated compounds belong to the class of decagonal approximant phases with stacked-layer crystallographic structure and show large structural complexity and the unit cell size.

The o -Al₁₃Co₄ and Al₁₃Fe₄ exhibit a positive-temperature-coefficient electrical resistivity typical of regular metals and alloys. The thermoelectric power change sign from negative, electron-like, to positive, hole-like, with the change of crystallographic direction. The anisotropic electronic transport coefficients were reproduced theoretically by an *ab-initio* calculation using Boltzmann transport theory and the calculated anisotropic Fermi surface. The T-Al_{72.5}Mn_{21.5}Fe₆ shows the non-metallic anisotropic electrical resistivity, which was analyzed within a unified theoretical approach of the Kubo-Greenwood response theory, where the central quantity is the spectral conductivity function that incorporates both the band structure of the system through the density of states, and the transport properties through the diffusivity. For the investigated compounds anisotropic thermal conductivities are the highest along the stacking direction. Common to all the investigated compounds is the fact that the stacking direction is the most conducting one for both the electricity and heat transport.

The investigated decagonal approximant phases exhibit anisotropic transport properties qualitatively similar to that of the *d*-Al-Ni-Co-type decagonal quasicrystals. The approximants and the *d*-QCs have both in common one set of structurally similar planes which are stacked periodically. The stacked-layer structure appears to be at the origin of the anisotropic transport properties, whereas the in-plane structural details seem to be of marginal importance for the anisotropic electronic transport properties of these stacked-layer intermetallic compounds.

FERMI-SURFACE EFFECTS IN ICOSAHEDRAL QUASICRYSTALS

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Icosahedral quasicrystals display low but nonzero density of the electronic states at the Fermi energy. In this sense these solids are metals and are expected to have the Fermi surface. Due to an interaction of the Fermi sphere with the boundaries of the pseudo Brillouin zone the Fermi surface of an icosahedral quasicrystal becomes nearly obliterated. The surviving fragments of the Fermi surface are very small electron-hole pockets. The fractional multicomponent Fermi-surface model that views the Fermi surface as consisting of a large number of very small pockets of electrons and holes separated by a distance which is much larger than the pocket size has been proposed for the band structure of icosahedral quasicrystals by Burkov and co-workers [1,2]. Independently, Fujiwara and co-workers [3], using the first-principles calculations of the electronic structure of cubic α -Al-Mn-Si, a 1/1 rational approximant of an icosahedral quasicrystal, have demonstrated that the Fermi surface of this compound contains several small electron and hole pockets, and mentioned the role of inelastic scattering in enhancing the electronic transport at high temperatures. Here we discuss the following predictions of the fractional Fermi-surface model at high temperatures, i.e., at the temperatures exceeding the Debye temperature: the power-law temperature variation of the electrical conductivity, the strong temperature variation of the thermal conductivity; the validity of the Wiedemann–Franz law, the excess electronic contribution to the specific heat, the appearance of a weak diamagnetism and the temperature variation of the electromagnetic response [4,5].

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ELECTRONIC PROPERTIES VERSUS LATTICE COMPLEXITY IN AL-BASED COMPLEX METALLIC ALLOYS

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In Al-based intermetallics, the interaction at the Fermi energy (E_F) between electronic states originating from aluminum and from transition elements plays a key role in the stabilization of these compounds. It has been assessed, both experimentally and theoretically, that stability is monitored by both the Hume-Rothery interplay between Fermi surface and Brillouin zone and sp-d hybridization at E_F , where sp states are basically brought by Al whereas d states essentially belong to the transition element. With a view at trying to understand better the balance between the two types of contributions, the paper will address two essentially different properties, namely friction against steel in vacuum and thermal conductivity, in order to investigate their scaling with the complexity of the lattice in a series of Al-based Complex Metallic Alloys. To this end, a simple index for complexity will be introduced. This index will be used to show that a similar scaling is observed along the formation of d-like states in the series of Al-Mg(-Zn) alloys made of elements that contain no d-states in their valence band before alloying.

THE FIBONACCI QUASICRYSTAL – NEW SURPRISES FROM AN OLD MODEL

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The Fibonacci sequence of *Long* and *Short* intervals on the one-dimensional line is a favorite textbook model for demonstrating the peculiar nature of electrons in quasicrystals. The wave functions of Fibonacci electrons are neither extended nor exponentially-localized, but rather decay algebraically; the spectrum of energies is neither continuous nor discrete, but rather singular-continuous, like a Cantor set; and the quantum dynamics is anomalous. In recent years we have studied how these three electronic properties change as the dimension of the Fibonacci quasicrystal increases to two and three, by constructing square and cubic versions of the Fibonacci quasicrystal.

We shall quickly review some of our findings, showing that whereas Fibonacci electrons in one dimension always behave as described above, in two dimensions, and even more so in three, there is crossover—as a function of the strength of the quasiperiodicity—to a regime in which Fibonacci electrons behave very much like electrons do in periodic crystals. More surprisingly, our studies of Fibonacci electrons have led us to new results also in the simple one-dimensional case. We shall describe two of these:

- (1) We have examined dynamical properties, such as the probability of an electron to remain in its original position as a function of time. The power-law decay of this quantity is a well-known and accepted parameter for analyzing the dynamics. Surprisingly, we have observed *log-periodic oscillations* on top of the power-law decay, implying the existence of an imaginary correction to the real exponent.
- (2) We have examined the extent of one-dimensional electronic wave functions in situation where there is a slight uncertainty in the exact electron energy, and much to our surprise we have observed the emergence of *quasiperiodic Bloch-like electronic wave functions*.

QUASIPERIODIC ANTIFERROMAGNET WITH PENTAGONAL LOOPS

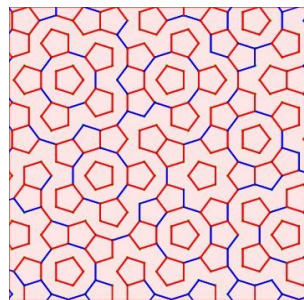
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In the context of magnetism, frustration arises when a group of spins cannot find a configuration that minimizes *all* of their interactions *simultaneously*. The simplest example is that of three spins placed on corners of a triangle. When the spins are classical Ising variables, and the couplings between pairs are antiferromagnetic, the configurations of lowest energy must have one frustrated bond since three spins cannot be mutually antiparallel. For Heisenberg spins, the ground state energy can be minimized by demanding that $\sum S_i = 0$, which leads to minimum energy states in which spins form 120° angles with respect to each other. In some lattices, this can lead to a macroscopic degeneracy of minimal energy states, with the possibility of new types of low temperature phases, the so-called spin liquids. This has led to a lot of interest over the recent years in spin systems based on triangular elements (the Kagome lattice, or the pychlore lattice, etc). We will present work generalizing the above considerations to structures with pentagons, or five-sided loops, which are also frustrated structures in the presences of antiferromagnetic interactions.

Five-fold loops are expected to arise naturally in quasicrystals and local five-fold symmetry is often manifest in experimental studies of surfaces of icosahedral or decagonal alloys. Our model considers classical Heisenberg spins placed on a subset of vertices of the two dimensional Penrose tiling, and interacting with nearest neighbors via antiferromagnetic bonds. The calculations were performed by Monte Carlo, on periodic approximants of the Penrose tiling. We address the issue of the energy, the degeneracy ground states of the infinite cluster, and the nature of low energy excitations. One of of the local spin configurations that minimize energy in this model is illustrated in the figure below. The results for this quasiperiodic antiferromagnet will be compared and contrasted with those of some other pentagonal periodic spin models.



Low energy configuration with bonds colored according to their energy (« singlets » in blue, and frustrated ($4\pi/5$) bonds in red)

MAGNETIC PROPERTIES OF Cd₆R 1/1 APPROXIMANTS

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Cd₆R (R=rare earth) compounds are bcc crystals composed of Tsai-type icosahedral clusters, which are regarded as one of the building units of stable binary quasicrystals Cd_{5.7}Yb and Cd_{5.7}Ca[1]. In view of the magnetic properties, these binary approximants are very attractive since they contain a magnetic element R except for Cd₆Yb and the position of the R atoms is fully determined by single-crystal X-ray structural analyses[2], i.e., they are exclusively situated at the second icosahedron shell and all the other sites are occupied by Cd atoms. The latter fact is in contrast to ternary systems where chemical disorder among constituent elements is essentially unavoidable, as manifested by their relatively wide single phase regions.

Hence, the Cd₆R compounds can be regarded as well-defined ideal spin systems, i.e., a bcc array of an icosahedron made of well-localized 4f spins. However, inherent to the lack of the chemical disorder, a single phase is obtained only at a certain stoichiometric composition close to Cd₆R, which makes preparation of a single phase very difficult. Therefore, synthesis of single grains is requisite for the investigation of the physical properties that are sensitive to foreign phases. In this work, single grains of Cd₆R were prepared for electrical and magnetic properties measurements. Single grains were grown in an alumina crucible sealed inside a quartz tube under Ar atmosphere by a self flux method. The single grains were then removed from the Cd melt using a stainless centrifuge by shuffling the quartz ampule at a high temperature and were further annealed to remove quenched-in defects introduced after shuffling.

The magnetic susceptibility measurements show that the susceptibility obeys the Curie-Weiss law above ~50 K for all the Cd₆R compounds investigated, showing a paramagnetic nature of 4f spins sitting on the vertices of the R₁₂ icosahedron. The obtained magnetic moments are almost the same as the theoretical values of the R³⁺ free ions, indicating that the R³⁺ ions are well localized in a trivalent state as in the cases of Cd-Mg-R quasicrystals[3]. The results of the low temperature measurements will be discussed in detail in the presentation.

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VALENCE FLUCTUATION STATE IN Yb BASED QUASICRYSTALS

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Recently, we found that intermediate-valence states are realized in the Yb-based quasicrystals under pressure. They form a new group of quasiperiodic system having a charge degree of freedom at each quasiperiodic lattice point.

As for an icosahedral Cd-Yb quasicrystal (*i*Cd-Yb), XANES experiments near Yb L_{III} -edge revealed that the Yb valence (ν) of divalent at ambient pressure increases continuously to 2.3 at 32 GPa. Although all Yb sites are crystallographically inequivalent each other, our comparison study to the crystalline approximant shows that *i*Cd-Yb at pressure can be considered as a quasi-periodic system of the identical Yb sites with respect to the charge degree of freedom. The continuous valence increase is interpreted as follows. The Yb 4*f*-level, slightly broadened due to the conduction *f*-electron hybridization, is gradually raised by compression because the initial 4*f*¹⁴ state of large ionic radius becomes less stable under pressure. Then, the 4*f*-level partially exceeds the Fermi level, and 4*f*-holes are generated. As the 4*f*-level is gradually raised, the 4*f*-hole number per Yb site (n_h) increases continuously, which means continuous valence increase because of the relationship; $\nu = n_h + 2$.

The electronic state of the intermediate-valence Yb compounds can be characterized by n_h , since the effect of the hole-hole repulsive interaction increases with the hole density. Since the present case is assigned to the lower n_h region of weak hole-hole correlation, *i*Cd-Yb under pressure is considered to take a valence fluctuation state which is described as a quantum superposition of the 4*f*¹⁴ and 4*f*¹³ state; $a|4f^{14}\rangle + b|4f^{13}\rangle$. Since this state would have large density of state (DOS) at Fermi energy in contrast to the already known quasicrystalline alloys having pseudogap electronic structure, new electronic properties are expected to be shown.

Further compression will shift *i*Cd-Yb to a heavy-fermion system in the strong correlation region ($\nu > \sim 2.7$). Here, a quasiperiodic charge order or charge glass transition can occur accompanied with valence transition due to changing 4*f*-hole character from the delocalized state to the localized one.

We also found that an icosahedral Cd-Mg-Yb quasicrystal takes an intermediate-valence state under pressure as well. The results will be applicable to other Yb-based quasicrystal.

LATTICE DYNAMICS IN COMPLEX ZINC-MAGNESIUM PHASES

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Dynamical properties of complex metallic alloys are closely related to their structure building motifs. The cubic $\text{Zn}_{11}\text{Mg}_2$ phase, a packing of Pauling triacontahedra linked by Zn octahedra, shows an intermediate structural complexity in between the Zn_2Mg Laves phase and the complex 1/1 approximant and quasicrystal $\text{Zn}(\text{Mg})\text{Sc}$. In a detailed comparison $\text{Zn}_{11}\text{Mg}_2$ and the relatively simple Frank-Kasper type hexagonal Laves phase Zn_2Mg are investigated, indicating the influence of structural complexity on dynamical properties in the Zn-Mg system.

Both ab initio calculations and molecular dynamics simulations using effective potentials, as well as experimental data from inelastic neutron scattering, constitute the basis of our analysis.

In the generalized vibrational density of states of $\text{Zn}_{11}\text{Mg}_2$ we find a significant departure from Debye's law with dispersionless modes at 5 meV, corresponding to a gap opening, whereas the vibrational spectrum of Zn_2Mg shows the typical behaviour of a close-packed structure, being dominated by acoustic modes up to 10 meV. While the dynamics in the Zn_2Mg Laves phase are well reproduced by ab initio simulation within the harmonic approximation, in $\text{Zn}_{11}\text{Mg}_2$ structural disorder is playing a crucial role, thus enforcing the molecular dynamics approach using EAM (embedded atom method) potentials. The processes, responsible for the exceptional excess of modes at low energies in $\text{Zn}_{11}\text{Mg}_2$, are studied by a detailed survey of eigenvectors, relating structural complexity and specific atomic motions to the GVDOS of this phase.

SURFACES OF ICOSAHEDRAL Cd-Yb FAMILY QUASICRYSTAL: STRUCTURE, ELECTRONIC PROPERTIES AND EPITAXY

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We will review our recent works on surface studies of the icosahedral (*i*) Ag-In-Yb quasicrystal, which is isostructural to the binary *i*-Cd-Yb phase. We employed a wide variety of experimental techniques including scanning tunneling microscopy (STM), medium energy ion scattering (MEIS), ultraviolet photoemission spectroscopy (UPS) and x-ray photoemission spectroscopy (XPS) to investigate the atomic structure, valence band, oxidation behavior of the high symmetry surfaces and their use as templates to grow thin films. The experimental results are compared with model structure and calculations.

The fivefold, threefold and twofold surfaces can be prepared with large terraces exhibiting symmetries expected from the bulk. With the STM results and the bulk structure of *i*-Cd-Yb, the terraces in the fivefold surface are identified at bulk positions which are dense and intersect the center of rhombic triacontahedral clusters, the building blocks of the system [1]. MEIS results are also consistent with the bulk model structure.

UPS reveals that the valence band near to the Fermi level is dominated by Yb 4*f*-derived states, in agreement with calculations [2]. As in the case of *i*-Cd-Yb, calculations yield a pseudogap in the density of states which is due to a hybridization of the Yb 5*d* band with the Ag/In 5*p* bands. The valence band is independent of the surface orientation. The elements in the quasicrystal are not distinct from pure elements Ag, In and Yb in terms of oxidation behavior in vacuum, air and water.

Among many elements deposited on the fivefold surface, Pb and Sb are found to be promising. Quasicrystalline Pb films can be obtained up to two atomic layers. The adsorption sites deduced from the STM images are in good agreement with potential energy calculations. After the completion of the second layer, fivefold twinned crystalline Pb islands of hexagonal symmetry are formed. These islands are of selective heights indicating electrons confinement in the islands. Pb islands are inert for adsorption of C₆₀ molecules, while quasicrystalline Pb bilayer shows strong interaction with the same molecules, as the clean surface does.

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**SURFACE SEGREGATION IN AN AL-BASED QUASICRYSTAL:
ZN IN DECAGONAL AL-PD-ZN**

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Surfaces of Al-rich quasicrystals seem to be generally stable against surface segregation. In cases where the surface composition has been reported to deviate from the bulk composition, the deviation has been small and has been inconsistent among different reports in the literature, so the situation has not been clear. However, we find that the situation is very clear for Al-Pd-Zn. We have studied the surfaces of this newly-discovered¹ decagonal phase with X-ray photoemission spectroscopy and scanning tunneling microscopy. Both twofold and tenfold surfaces are very rough after sputtering and annealing, and cannot be prepared in a terrace-step morphology. This is due to preferential segregation of Zn, and evaporation of Zn at relatively low temperature (detectable in the gas phase at 600 K). Evaporation restricts the temperature at which the samples can be annealed.

We conclude that Zn is bonded weakly in the quasicrystal, perhaps as weakly as in elemental Zn. This conclusion is based not only upon the observation of surface segregation, but also two others: (1) The vapor pressure of Zn above the quasicrystal is comparable to that expected for elemental Zn; and (2) During sputtering, Zn is removed preferentially—which is contrary to the usual preferential sputtering of Al in Al-rich quasicrystals.

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Cu ADSORPTION ON THE (100) SURFACE OF THE $\text{Al}_{13}\text{Co}_4$ APPROXIMANT

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Quasicrystal surfaces have intensively been used as templates for the growth of thin metallic films [1]. Among the numerous systems reported, the adsorption of Cu atoms on icosahedral surfaces has led to the formation of a 1-dimensional aperiodic thin film [2] and to the growth of complex surface alloys [3-4]. The recent growth of centimeter-sized approximant samples [5] allows the direct comparison of growth phenomena on related periodic and aperiodic surfaces. To this end, we have used the p -10f surface of the orthorhombic $\text{Al}_{13}\text{Co}_4$ crystal as a template for the adsorption of Cu thin films of various thicknesses deposited at different temperatures. From 300 K to 573 K, Cu adatoms grow pseudomorphically up to one monolayer. At 300 K, the β -Al(Cu,Co) phase appears for coverages greater than one monolayer. For higher temperature deposition, the β -Al(Cu,Co) phase is followed by the formation of the γ - Al_4Cu_9 phase. Both β and γ phases grow as two (110) domains rotated by 72° from each other. The orientations of the bipentagonal motifs present on the clean $\text{Al}_{13}\text{Co}_4$ (100) surface dictate the growth orientation of these domains. The initial bulk composition and structural complexity of the substrate have a minor role in the formation of the γ - Al_4Cu_9 phase as long as the amount of Al and the Cu film thickness reach a critical stoichiometry.

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CATALYTIC PROPERTIES OF $\text{Al}_{13}\text{Co}_4$ STUDIED BY *AB INITIO* METHODS.

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Surfaces of quasicrystals and their approximants can have interesting catalytic properties. While the surfaces of ordinary crystals provide only a few inequivalent adsorption sites, the complex landscape of quasicrystalline surfaces provides a rich variety of different adsorption sites and possible catalytic reactions pathways. Acetylene hydrogenation is a subprocess at the industrial production of the polyethylene. This process is generally carried out using Pd catalyst. The possibility to replace an expensive Pd by an Al-based transition-metal alloy is highly intriguing. Recently Armbrüster et al. [1] reported that the complex intermetallic compound $\text{Al}_{13}\text{Co}_4$ is an efficient and selective hydrogenation catalyst for alkynes. In the present contribution the hydrogenation of acetylene to ethylene on the surface of $\text{Al}_{13}\text{Co}_4$ has been studied using *ab initio* density-functional method. The surface of $\text{Al}_{13}\text{Co}_4$ decagonal approximant is very peculiar. The structure of the surface consists of islands of two connected Al pentagons, each centered by a Co atom. Binding energies for adsorption and coadsorption of H_2 and C_2H_2 molecules at various sites on the surface were calculated. The initial step of the reaction is the dissociation of the H_2 molecule. We have searched for and explored optimal reaction pathways for C_2H_2 hydrogenation by the Langmuir-Hinshelwood mechanism. The hydrogenation is an exothermic multi-step process where C_2H_2 is first transformed to C_2H_3 and then C_2H_3 to C_2H_4 . The energetic barriers of the reaction steps were calculated by the nudged-elastic-band method. It was found that the energetic barrier of any reaction step does not exceed 0.7 eV (68 kJ/mol). This value is lower than the height of the energetic barrier at the acetylene to ethylene hydrogenation over the Pd catalyst where for the rate determining step the barrier heights between 78 kJ/mol and 85 kJ/mol were reported.

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Topological invariants of aperiodic tilings

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Every aperiodic tiling is a member of an infinite class of tilings which are locally indistinguishable from each other. Such an LI class of tilings can be given a natural topology, making it a compact topological space. The resulting tiling spaces (spaces whose points are tilings) have interesting topological properties, which reflect properties of the underlying tilings. For important classes of tiling spaces, certain topological invariants, especially the Čech cohomology groups, can explicitly be computed. In particular, this is the case for primitive substitution tilings and canonical projection tilings. The key for these computations is a systematic approximation of the tiling spaces by simpler spaces, finite cell complexes, for which the cohomology can be computed by elementary means. In this talk, we shall give an overview on these results, explaining the main ingredients in simple terms.

DETERMINING QUASICRYSTAL STRUCTURE ON SUBSTITUTION TILINGS

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Quasicrystals are characterized by the diffraction patterns which consist of pure bright peaks. Substitution is quite a commonly used method to create geometrical models for quasicrystals. We consider substitution tilings and show how to determine quasicrystalline structure computationally. In order to complete the computation, it is important to have the Meyer property on the substitution tilings. We also show how to check the Meyer property on the substitution tilings from the expansion map of the substitution.

COLOURINGS OF LATTICES AND CSLS

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Coincidence site lattices (CSLs) and coincidence site modules (CSMs) are an important tool to describe grain boundaries in crystals and quasicrystals. They are closely related to colourings of lattices. In particular, colourings can be used to solve the coincidence problem for a sublattice, once the coincidence problem has been solved for its parent lattice. We review this relationship and discuss new developments on this topic. That is, we discuss the relationship between the coincidences of shifted lattices and colour coincidences and how they can be used to compute the coincidence indices of sublattices.

**COLOURINGS OF CYCLOTOMIC INTEGERS
WITH CLASS NUMBER ONE**

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This work continues the study on symmetries pertaining to colourings of cyclotomic integers [PC]. The study investigates ideal colourings (q) of $\mathcal{M}_n = \mathbb{Z}[\xi_n]$ (where $\xi_n = e^{2\pi i/n}$ is a primitive n th root of unity) for values of n for which $\mathbb{Z}[\xi_n]$ is a principal ideal domain and thus has class number one. The values of n are grouped into classes with equal value of $\phi(n)$, the Euler's totient function. Our previous work derived the colour symmetry group H for any n and focused on determining the colour preserving group K for the crystallographic cases: $n = 3, 4$; as well as the non-periodic cases: $n = 5, 8, 12$ (involving standard quasicrystallographic symmetries) and $n = 7, 9$. In this note, results on K are enumerated for the cases $n = 11, 15, 16, 20, 24$; thus completing the characterization of colour symmetries of ideal colourings associated with \mathcal{M}_n for $\phi(n) \leq 10$. For the rest of the values of n for which \mathcal{M}_n has class number one, we provide a methodology to list all the indices of (q) in \mathcal{M}_n for which K is trivial. Furthermore, an ideal colouring (q) of \mathcal{M}_n may be manifested geometrically as a vertex or tile colouring of a two dimensional tiling with n -fold rotational symmetry, which is non-periodic for $\phi(n) > 2$. For such cases, since \mathcal{M}_n is dense on the plane, we choose a discrete subset of \mathcal{M}_n for which we show the colours.

[PC] E.P. Bugarin, M.L.A.N. de las Peñas, D. Frettlöh: Perfect colourings of cyclotomic integers
[in print, 0905.4048]

POINT SUBSTITUTION PROCESSES FOR GENERATING ICOSAHEDRAL TILINGS

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The use of inflation rules (IRs) has culminated in the discoveries of a variety of *quasiperiodic tilings* (QTs) that can be found in the literature. To name a few are several two-dimensional (2D) QTs such as the Penrose and the Stampfli tilings, while the 3D icosahedral QT (IQT) by Danzer is also on the list. However the discoveries of these QTs have so far been made by trial and error, and hence the list is rather restrictive. A more systematic use of IRs needs to be pursued in exploring the whole range of possible QTs, which would then provide us with an abundance of geometrical models that can be used to describe real quasicrystals. This serves also to understand the relationships between different structures and moreover the origin of their stability in real systems. It is only recently that IRs have been formulated into a systematic scheme for generating quasilattices (QLs), which implies a Delone set (i.e., a point set which is uniformly discrete and relatively dense). The scheme is called *point inflation rules* [1] and has proved to be useful for generating many unknown QLs at the cost of moderate effort; it has also been applied to icosahedral QLs as well [2, 3]. With a modification of the basic toolset, a systematic inflation scheme for constructing 2D QTs has also been proposed [4]; the scheme is called *generalized point substitution processes* and has been applied to generating new families of decagonal QTs[4, 5]. In this paper, the new scheme is extended to generating 3D IQTs. Several well known IQTs including the 3D Penrose tiling as well as the T^{2F} tiling by Kramer, which have been discovered via the projection formalism, can also be generated by the present scheme. The shapes of the windows for these prototypal IQTs are polyhedral, while from the analogy of the 2D case it is highly likely that there exist many more IQTs which have windows with fractal boundaries. An attempt to construct such IQTs, including a possible IQT whose prototiles are the four *canonical cells* [6], is made, and the latest results will be discussed at ICQ11.

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RANDOM POINT SETS AND THEIR DIFFRACTION

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The diffraction of random subsets of the integer lattice \mathbb{Z}^d , such as the coin tossing sequence, are well understood. Here, we go one important step beyond and consider random point sets in \mathbb{R}^d . We present various systems with an effective stochastic interaction that still allow for explicit calculations of the autocorrelation and the diffraction measure. We concentrate on one-dimensional examples for illustrative purposes, and briefly indicate possible generalisations to higher dimensions.

In particular, we discuss the stationary Poisson process and the renewal process on the line. The latter permits a unified approach to a rather large class of one-dimensional structures, including random tilings. Moreover, we present some stationary point processes that are derived from the classical random matrix ensembles as introduced in the pioneering work of Dyson and Ginibre. Their re-consideration from the diffraction point of view improves the intuition on systems with randomness and mixed spectra.

THE STRUCTURE OF DECAGONAL Al-Ni-Co SUPERSTRUCTURE TYPE I

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During last several years the phase diagram of Al-Ni-Co has been thoroughly investigated. There are eight different decagonal phases reported in this system [1 and references therein]. One of them is the so called superstructure type I phase (also known as the Edagawa Phase, discovered by Edagawa et al. in 1992 [2]). No qualitative structure analysis of this phase has been performed yet.

The diffraction pattern of the superstructure type I phase consists of strong main reflections and rather weak satellite reflections. The satellite reflections cannot be indexed in the standard decagonal reciprocal lattice basis. Instead one has to use a rotoscaled basis [3] (rotated by an angle of $\pi/10$ and rescaled by the factor of $(3 - \tau)^{1/2}$).

We present the first refinement results of the Edagawa Phase conducted in the physical space. The structure factor, which was used for the modelling process, was calculated on the basis of a statistical approach described in [4,5], which allows a purely 3-dimensional, real space optimization of a quasicrystalline structure. A large synchrotron data set was merged in 10/m Laue group yielding 6141 symmetrically independent reflections (1317 main and 4824 satellite). The structure model was derived from electron density maps obtained by the charge flipping method. Our structure units are thick and thin rhombuses of the Penrose tiling (edge length $a \approx 19\text{\AA}$), whose vertices are decorated by a decagonal cluster. This model is almost consistent with the one proposed by Yamamoto and Weber [6].

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SUPERSTRUCTURE DETERMINATION OF BASIC Co-RICH DECAGONAL Al-Co-Ni

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The superstructure of the high-temperature phase of basic Co-rich d-Al_{72.5}Co_{18.5}Ni₉ with a double period along the ten-fold direction has been determined based on single-crystal x-ray diffraction data. The x-ray diffraction pattern of this structural modification has very peculiar extinction conditions. Previously, a higher dimensional model with color symmetry has been proposed to explain the similarly peculiar extinction conditions that have been observed for the d-Al-Ni-Fe structure [1]. For the structure of interest here, this approach is insufficient to correctly account for the experimentally observed intensity distribution. Using as a starting model the average structure of the d-Al_{72.5}Co_{18.5}Ni₉ phase that was determined in our previous work [2], we use a special mode analysis together with a five-dimensional non-centrosymmetric space group $P\bar{1}02c$ to obtain the observed peculiar extinction conditions. The five-dimensional structure model was refined with 300 parameters, $wR = 0.06$ and $R = 0.21$ for 1220 reflections. The close relationship of the model structure with that of W-Al-Co-Ni, a $\langle 3/2, 2/1 \rangle$ -approximant, is shown.

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POINT-DEFECT DISTRIBUTIONS IN AN IDEAL $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ STUDIED BY ULTRAHIGH-RESOLUTION STEM AND FIRST-PRINCIPLE CALCULATIONS

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Phason is a unique elastic degree of freedom specific for quasicrystals, causing atomistic fluctuations at particular atomic sites. Quantitative analysis of these phason-related point defects is important to understand phason-related atomistic behaviors in the quasicrystals. In the present work, we use aberration-corrected ultrahigh-resolution scanning transmission electron microscopy (STEM) to indentify the occupations of individual atomic sites in the decagonal $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, which is one of the best quasiperiodically ordered materials available today. We further attempt to evaluate a stability of several phason-related local configurations based on first-principle energy calculation using Vienna *Ab-Initio* Simulation Package (VASP).

We indeed find that significant point defects occur even for the highly ordered $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, the localized distribution of which is well represented by the decagonal cluster located at the quasilattice with a length-scale of 2nm. For each of the clusters, phason-related disorders are found to be significant around the core of the clusters, and the detailed disorder configurations appear to be slightly different between the clusters. However, a striking intensity map has emerged after simply summing the local cluster intensities by concerning their polarity in accordance with the Penrose vertex symmetry; the averaged cluster turns out to possess definite mirror symmetry (Fig. 1). This strongly implies that the defect occurrences are well governed by the underlying Penrose tiling symmetry. We presume that the intrinsic vacancies at the Al sites around the cluster core plays a key role for local phason-related dynamical behaviors, which might lead to a long-wave phason mode. Vacancy-induced change of local atomic configurations will be discussed with the aid of first-principle energy calculations.

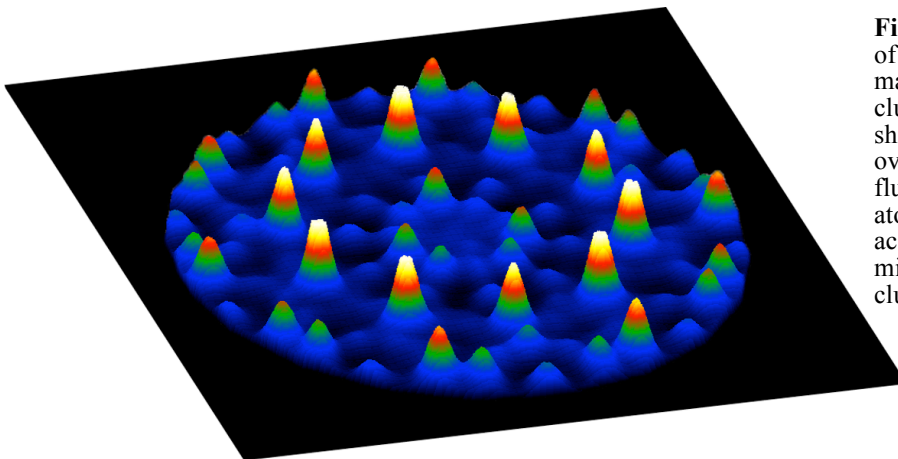


Fig. 1 3D representation of the average intensity map of the decagonal clusters in $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$, showing clearly that overall composition fluctuations at individual atomic sites are in good accordance with average mirror symmetry of the cluster.

CORRELATING THE LOCAL DENSITY OF STATES AND THE MACROSCOPIC CONDUCTIVITY IN QUASICRYSTALS AND APPROXIMANTS

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Quasicrystals (QC) show very particular mechanic, magnetic and electronic properties which differ markedly from their constituent elements. In particular, the very high electrical resistivities which even show negative temperature coefficients and the residual resistivities of QC, which increase with the quality of the samples. Not only QC possess such remarkable physical properties, but also their periodic counterparts, the approximants or even other large unit cell alloys. The origin of these special physical properties as well as the stability of these systems is based on the valence electronic structure. Two main characteristics in the density of states (DOS) of such complex metallic alloys (CMA) are apparent:

- Pseudo gap ($\sim 1\text{eV}$) around the Fermi Energy due to Hume-Rothery stabilization
- Localized electrons evidenced by a Spiky local DOS

Theoretical investigations of the electronic resistivity consider both characteristic features of the DOS of CMA, the depletion at E_F and the localization of electrons [1]. However, which of the two features is crucial (or even both) for the unusual electrical resistivity of CMA is a still an open question. In this presentation we discuss the correlation between the variation in the local DOS determined by Scanning Tunneling Spectroscopy and the electrical resistivity as displayed in Fig. 1. A clear impact of the local spikiness and the structural complexity on the global electrical resistivity is revealed.

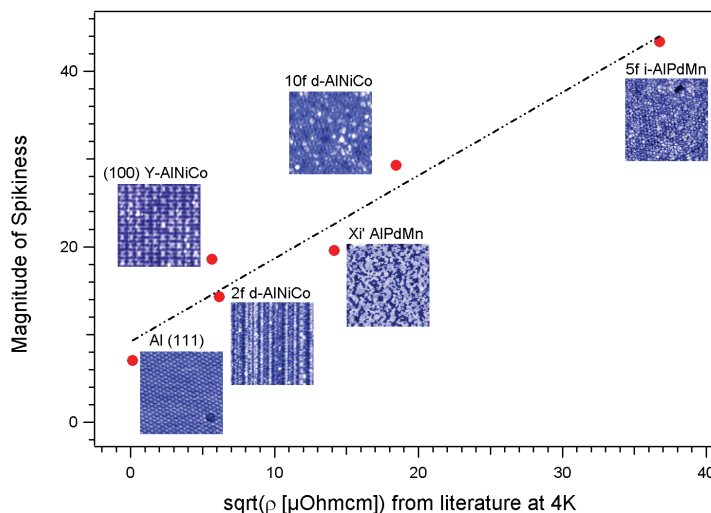


Figure 1: Correlation between local variations in the Density of States and the electrical resistivity

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METAL INSULATOR TRANSITION INDUCED BY LONG RANGE QUASIPERIODIC ORDER IN OCTAGONAL TILING

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The understanding of the remarkable transport properties of quasicrystals is a long standing question that still does not have a definite answer. It has been shown that medium range quasiperiodic order in AlMn, AlCuFe and AlCuCo quasicrystals leads to an “insulator like” behavior [1,2]. In one dimensional quasiperiodic tilings, critical states have been found showing a new type of electron localization. A major question is whether these states persist in higher dimension. Up to now very few quantum transport calculations have been performed for two- and three-dimensional quasiperiodic tilings (see in particular [3,4]). Triozon et al. [4] have shown a non-ballistic regime in generalized Rauzy tilings, but with metallic conduction.

Here we investigate electronic quantum transport in a two dimensional octagonal tiling [5] by using the M.K.R.T. (Mayou-Khanna-Roche-Triozon) method [3,4]. For the first time we show that long range quasiperiodic order induces a sub-diffusive regime at some energies. Therefore, a small shift of the Fermi energy can cause a system without defects to undergo a Metal-Insulator transition. These results are obtained for a pure hopping Hamiltonian (one type of atom) and for model Hamiltonians that simulate different types of atom.

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ENHANCING THE CRITICAL CURRENT IN SUPERCONDUCTORS WITH QUASIPERIODIC PINNING ARRAYS BELOW AND ABOVE THE MATCHING FLUX

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The increase of the critical current is one of the main goals of applied superconductivity. The motion of vortices, driven by an external current in type II superconductors leads to the energy dissipation and thus to the deterioration of the superconducting properties. The critical depinning current J_c can be enhanced by trapping vortices by pinning centers. Recent progress in fabrication of nanostructures has provided a wide variety of well-controlled vortex confinement topologies, including different regular arrays of pinning sites (APS). Periodic APS are efficient for matching flux Φ_1 (and $n\Phi_1$, where n is an integer) corresponding to one trapped vortex per pinning site resulting in a sharp peak in J_c . However, this peak in J_c is too narrow and not robust against changes in Φ .

The critical depinning current $J_c(\Phi)$ in one-dimensional quasiperiodic chains and two-dimensional APS placed on the vertices of a five-fold Penrose tiling, was first theoretically studied in [1]. Comparing the J_c 's for QP (Penrose-tiling), periodic and random APS, it was found that the Penrose-tiling provided a broad maximum in the critical current $J_c(\Phi)$. The theoretically predicted broad peak in $J_c(\Phi)$ was verified in experiments with APS of antidots [2] and magnetic dots [3] placed on the vertices of the Penrose tiling. However, while regular APS showed only a sharp peak in $J_c(\Phi)$ for the matching flux Φ_1 and QP APS provided a much broader maximum at $\Phi < \Phi_1$, both types of pinning arrays turned out to be inefficient for fluxes larger than Φ_1 [4, 5]. We demonstrate [6] theoretically and experimentally the enhancement of $J_c(\Phi)$ for $\Phi > \Phi_1$ by using QP pinning arrays other than Penrose-tiling. This result is based on a qualitatively different mechanism of collective flux pinning and could be useful for practical applications demanding high J_c 's over a wide range of fields.

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BRITTLE FRACTURE OF A COMPLEX METALLIC COMPOUND FROM AN ATOMISTIC VIEWPOINT

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Material-specific atomistic aspects of brittle fracture are studied for the first time for a complex metallic compound with realistic embedded-atom-method potentials. Crack propagation occurs on an atomic level by a successive rupture of cohesive bonds. In many theoretical models of fracture, however, a coarse-grained approach is applied and the explicit influence of the discrete nature of matter is not taken into account. In this talk, numerical experiments on the complex metallic compound NbCr₂ are presented to illustrate why it is necessary to perform atomistic simulations to understand details of fracture behaviour: The number, strength and orientation of bonds approached by a crack determine whether, where and how it propagates [1].

Fracture of a three-dimensional brittle solid generates two-dimensional surfaces, which are formed behind a one-dimensional crack front. For quasi-static cracks on a (111) cleavage plane in silicon front propagation by kink-pair formation was proposed and proven by a reaction-pathway analysis with Stillinger-Weber potentials [2]. Here, we demonstrate that the kink-pair mechanism is much more general: We also observe it in molecular dynamics simulations of the C15 NbCr₂ Friauf-Laves phase. The numerical experiments highlight that kink formation is essential for crack propagation in any brittle material [3].

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MG-ZN-AL ALLOYS CONTAINING QUASICRYSTAL AND RELATED PHASES FOR STRUCTURAL APPLICATIONS

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Magnesium alloys have great potential as structural materials because they are the lightest of all structural alloys in industry. To be used in structural applications, the alloy's mechanical properties, i.e., strength, ductility and toughness, must be sufficient to satisfy both reliability and safety requirements. The quasicrystal phase occurs in equilibrium with the magnesium phase, showing a definite orientation relationship and with a strong interface, and this phase does not become the void nucleation site but has a role of pinning effect of dislocation movements. Thus, the dispersion of the quasicrystal phase into the magnesium matrix causes to enhance the mechanical properties; however, all these magnesium alloys contain rare earth (RE) elements to form the quasicrystal phase, which become problematic from economical and ecological points of view. In this study, the quasicrystal and related phase particles were successfully dispersed in the homogeneous and fine-grained structures by controlling the additional elements and processing, i.e., heat treatment. The present alloy also showed the good mechanical properties, which were the superior to that in the conventional Mg alloys and Mg-Zn-RE alloys with quasicrystal phases, and had an excellent secondary formability.

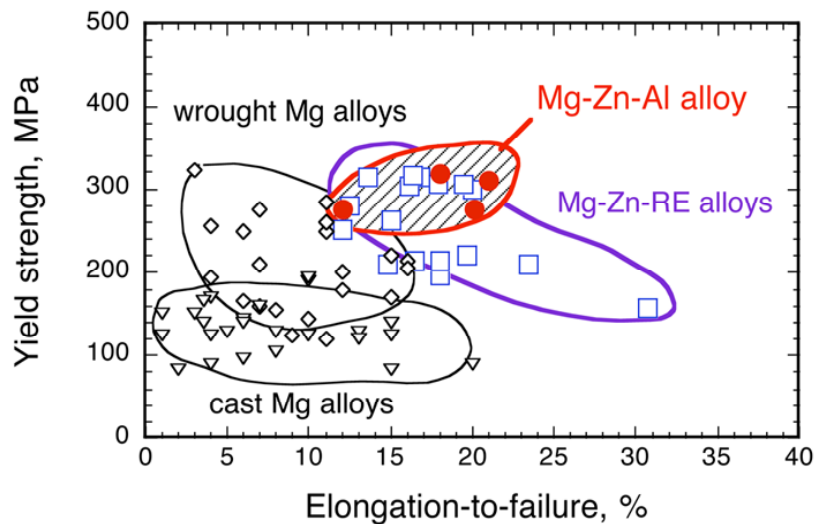


Figure: Relationship between yield strength and elongation-to-failure at room temperature in Mg-Zn-Al alloys and conventional magnesium alloys.

PREPARATION AND WEAR RESISTANCE OF Ti-Zr-Ni QUASICRYSTAL
AND POLYAMIDE COMPOSITE MATERIALS

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Ti-based icosahedral quasicrystals, discovered in 1985, have some unique physical/mechanical properties due to their extraordinary crystallographic structure. These properties, such as low surface energy, low friction coefficient and high stiffness, have made them ideal materials for evaluation as reinforcing fillers in metallic or polymeric materials. Polymer-metal composite materials are increasingly important due to their remarkable properties based on the combination of two different materials, and due to easy machinability of polymers. In order to achieve higher properties for specific applications, research is carried out in developing all kinds of fillers to improve the properties of polymers. Ti-Zr-Ni quasicrystal powders (QC), prepared by mechanically alloying and then annealing in vacuum furnace, were used as a novel filler material in polyamide 12 (PA12). The melt processability of the composite was studied using a Haake torque rheometer and a dynamic rotational rheometer and it suggests that PA12/QC composite can be melt-processed into a wear-resistant material. Further, this composite, fabricated by compression molding, was sliding against a polished metallic counterface. The results from wear testing showed that adding an appropriate amount of Ti-Zr-Ni quasicrystal filler in PA12 would enhance wear resistance as compared to unfilled PA12. The reduction in wear is explained in terms of the wear mechanisms. These results suggest that Ti-Zr-Ni quasicrystal filler may be a desirable alternative when attempting to increase the wear resistance of PA12 for applications.

Selective laser sintering of quasicrystalline preforms: A new technological application for manufacturing functional Al-based parts.

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Selective Laser Sintering (SLS) is a rapid prototyping technology used for building prototype parts from 3D computer-aided design (CAD). This technique allows fabricating complex geometry parts in a layer by layer fashion, with no need to use tools or dies. While SLS is typically used to produce parts consisting of a polymer based composite, it can also produce functional metal parts using a two step process. First a metal or an alloy (e.g. steel) and polymer binder powders are sintered by SLS to produce a rigid preform. Then the polymer binder is removed and replaced through infiltration of the preform by another metal (e.g. brass). While this process is well controlled for steel parts infiltrated with brass, all attempts to extend this process to low-weight materials have failed so far. Here we will show that quasicrystalline materials, more generally, Al-based complex metallic alloys can be used to produce Al infiltrated preforms via indirect SLS, resulting in fully dense, complex functional devices characterized by a low specific mass ($\sim 4 \text{ g/cm}^3$) as well as attractive mechanical properties [1].



Figure: An example of preform with complex geometry produced by SLS. The preform contains i -AlCuFeB quasicrystalline powders and can be infiltrated with liquid aluminum.

In this presentation, we will describe the SLS process, the previous attempts to develop its application to low-weight Al materials, and its causes of failure. Then we will discuss the reason why using quasicrystals allows us to circumvent the various problems previously encountered. This work opens a new direction for applications of quasicrystalline alloys and for the development of the SLS process towards a new class of light materials.

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A NOVEL CATALYST FABRICATED FROM Al-Co-Ni DECAGONAL QUASICRYSTAL FOR STEAM REFORMING OF METHANE

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Preparation, characterization and catalytic properties of novel catalysts made by leaching of stable decagonal quasicrystal, Al-Co-Ni (ACN) in dilute NaOH solution are reported here. The decagonal quasicrystal is stable over the wide range of composition of varying Co and Ni content. It has been found that leaching of ACN in dilute NaOH solution leads to formation of different phase mixture depending on the composition of precursor ACN. For Al₇₂Co₂₀Ni₈, the leached product consists of biphasic nanocrystals of hcp Co and fcc Ni where as for Al₇₂Co₁₄Ni₁₄ and Al₇₂Co₈Ni₂₀ precursors, leaching leads to formation of fcc α -(Co,Ni) nanocrystals. The composition of the α phase can also be tailored using different compositions of the precursor, and thereby the catalyst chemistry can be changed. The steam reforming of methane (SRM) has been performed on the catalysts to bring about the different behaviour of the catalyst. The results suggest that the alloying has a strong effect on the catalytic activity with Co:Ni=1:1, showing the best performance. The catalysts are found to be very stable against sintering at high temperature during SRM reaction. The results are compared with standard Raney Ni and Co catalysts. The results are discussed in light of available literature. Energy filter TEM (EFTEM) analysis has been carried out to show that the distribution of Co, Ni in the nanocrystals to show the difference in catalytic activity.

**SYNTHESIS OF POROUS Cu THIN FILMS FROM RF SPUTTERED
QUASICRYSTALLINE Al-Cu-Co ALLOY THIN FILMS**

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Miniaturization of chemical device necessitates the development of micro-reactor to replace conventional bead-pack techniques. In such micro-reactor, reaction occurs within the pores of thin film of the catalytic material. The Cu-rich porous films were obtained from Al-Cu-Co decagonal quasicrystalline phase by dealloying method, to understand the mechanism involved in the catalytic properties of this material. The Al-Cu-Co quasicrystalline alloy target was prepared by using arc melting machine. By using this target, decagonal Al₆₅Cu₂₀Co₁₅ thin films were prepared by using rf magnetron sputtering technique on SiO₂ and γ -Al₂O₃ substrates with thickness of about ~1500 nm. The dealloying of Al and Co was obtained after immersion of the sample in NaOH alkali solutions of about 3 hours, which leads to the formation of porous structure. The structural properties of the target and Al-Cu-Co thin film metal alloy were characterized by X-ray diffraction technique (XRD) and Scanning electron microscopy (SEM). The surface area of the porosity as measured by BET method was about 50 m²/g and the further analyses will be presented in detail.

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Development of thermal rectifier using the unusual electron thermal conductivity of quasicrystals

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By considering the unusual electron thermal conductivity caused by the narrow pseudogap at the Fermi level, we propose, in this paper, a new strategy to develop a thermal rectifier usable at high temperature above 300 K.

Recently, a new idea of thermal rectifier using two solid materials is proposed from both theory and experiment. [1,2] The thermal conductivity of one material in the rectifier increases with increasing temperature, while that of the other decreases. In order to realize this condition, Kobayashi *et al.* [1] proposed a use of the temperature dependence of lattice thermal conductivity expected for the well-ordered crystals and that of the disordered ones. The former materials possess lattice thermal conductivity that decreases with increasing temperature due to the decrease of phonon mean free path, while the latter increases due to the effect of the increasing specific heat of phonons. Although this is very interesting idea to realize a new thermal rectifier, the proposed devices can be used only at very low temperature because the thermal conductivity of both materials becomes constant at high temperature.

In sharp contrast to the lattice thermal conductivity, the electron thermal conductivity drastically increases with increasing temperature, provided that a narrow pseudogap persists at the Fermi level such as that in the the quasicrystals and approximants. Indeed the thermal conductivity of the typical Al-based icosahedral quasicrystals increase with increasing temperature, and its magnitude at 1000 K becomes almost one order larger than that at 300 K. By considering that the thermal conductivity of many metallic materials moderately decreases with increasing temperature at the temperature range above 300 K, we employed, in this study, Al₆₂Cu_{25.5}Fe_{12.5} quasicrystal and Al-Cu-Fe inter-metallic compounds to construct a new thermal rectifier consisting of these two compounds.

The single phased samples were prepared by the induction melting. After grinding the ingots into powder, we sintered powders into the bulk consisting solely of the objective phase by means of spark plasma sintering (SPS) method. By measuring temperature dependence of thermal conductivity, we determined the inter-metallic compound that is most preferable for the component of thermal rectifiers. The thermal rectifier consisting of icosahedral quasicrystal and the identified inter-metallic compound was also prepared by the SPS method.

In the presentation, the possibility of the newly developed thermal rectifier will be discussed in detail together with the mechanism leading to the drastic enhancement of electron thermal conductivity with increasing temperature.

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**THERMAL STORAGE OF DIGITAL INFORMATION IN THE
TAYLOR-PHASE DECAGONAL APPROXIMANTS**

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The Taylor-phase $T\text{-Al}_3\text{Mn}$ decagonal approximant and its solid solutions with Pd and Fe, $T\text{-Al}_3(\text{Mn,Pd})$ and $T\text{-Al}_3(\text{Mn,Fe})$, belong to the class of magnetically frustrated spin systems that exhibit rich out-of-equilibrium spin dynamics in the nonergodic phase below the spin-freezing temperature T_f . Performing large variety of magnetic experiments as a function of temperature, magnetic field, aging time t_w and different thermal histories, we have investigated the memory effect (a state of the spin system reached upon isothermal aging can be retrieved after a negative temperature cycle) and "rejuvenation" (small positive temperature cycle within the nonergodic phase erases the effect of previous aging) [1]. The memory effect lead us to propose a novel concept of a new kind of memory element, *a thermal memory cell*, where a byte of digital information can be stored into the storage material by pure thermal manipulation [2]. Thermal inscription of information employs a specific temperature–time profile that involves continuous cooling and isothermal waiting time periods in the absence of any external magnetic or electric field. We succeeded to thermally write arbitrary ASCII characters, representing text in computers, into the Taylor-phase $T\text{-Al}_3(\text{Mn,Fe})$ complex intermetallic compound. Besides for the data storage, the concept of a thermal memory cell may be employed for secure data transfer and for retrieving cosmological information from extraterrestrial dust particles.

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Negative refraction and localized states of classical wave in high-symmetry quasicrystals

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Abstract

Recently, negative refraction of electromagnetic waves in periodic photonic crystals was demonstrated experimentally and subwavelength images were observed. In this presentation, we report some theoretical and experimental investigations on the electromagnetic wave transport in high symmetry photonic quasicrystals (PQCs). It is shown that the negative refraction can appear in these transparent quasicrystalline photonic structures. It is interesting that the high symmetric two-dimensional PQC slabs possess universal feature for non-near-field focus of two kinds of polarized waves (S wave and P wave). That is to say, the non-near-field focus for two kinds of polarized waves can be realized by using the flat lenses, which are consisting of some high-symmetry two-dimensional PQCs with the same structures and parameters. In addition, some two-dimensional and three-dimensional localized states in defect-free PQCs have been found. It has been evident that these unusual localized states can be explored by means of the electron energy loss spectroscopy.

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Gamma-brass superstructures, perpendicular pseudo-5-fold axes, and the E8 lattice

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Many of the most common cubic intermetallic structures (MgCu_2 , Cu_5Zn_8 , Ti_2Ni , and $\alpha\text{-Mn}$) have superstructures with up to 400 atoms in their unit cell. These large superstructures ($\text{Li}_{21}\text{Si}_5$, $\text{Sm}_{11}\text{Cd}_{45}$, and $\text{Mg}_{44}\text{Ir}_7$) have perpendicular pseudo 5-fold axes. These pseudo 5-fold axes prove to be the result of a three-dimensional projection of the 600-cell four-dimensional Platonic point group. Such 4-D point groups are themselves embedded in the closest-packed eight-dimensional Bravais lattice, E8.

This situation is analogous to the 3-D icosahedral point group being embedded in a 6-D lattice, familiar amongst quasicrystals. We find that the above 3-D complex metal alloy superstructures are 3-D rational projections of the E8 lattice. The possibility of an irrational quasicrystalline 3-D projection is discussed. Finally, LDA-DFT parameterized tight-binding calculations are used to understand the stability of these phases.

MODULATED STRUCTURES OF LOW-DIMENSIONAL ELECTRONIC AND MAGNETIC CRYSTALS

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Aperiodic crystals are crystalline matter, because their structures possess—in principle—perfect long-range order, while lacking three-dimensional translational symmetry. Three kinds of aperiodic order are presently recognized: quasicrystals, incommensurate composite crystals, and incommensurately modulated crystals [1].

Important classes of compounds with incommensurately modulated structures encompass those with a one-dimensional electronic system [2]. They include organic charge-transfer salts, like TTF-TCNQ, and transition metal chalcogenides and oxides, like NbSe₃ and the blue bronze K_{0.3}MoO₃. Recent examples are the low-dimensional magnets MOCl ($M = \text{Ti, V, Cr}$) [3], and the CDW compounds Er₅Ir₄Si₁₀ and SmNiC₂ [4] with strong interchain coupling. The presence of large overlaps between valence orbitals on neighboring sites into only one direction has important consequences for the physical properties of these compounds. Phase transitions are often found towards states with charge-density waves (CDW), spin-density waves (SDW), the spin-Peierls (SP) state or spiral magnetic order. They may involve incommensurate or commensurate superstructures, depending on the Fermi wave vector and the frustration between electronic and elastic energies. These states are in competition with superconductivity (SC) and states with ferromagnetic (FM) or antiferromagnetic (AF) order.

Recent developments in the crystallography of aperiodic crystals include the superspace approach to magnetic superstructures [5]. Furthermore, there is an increasing recognition, that the superspace concept may help our understanding of what actually are simple superstructures, *i.e.* commensurately modulated structures.

Here, the implications are discussed of the (in)commensurate superstructures of low-dimensional electronic crystals for the understanding of these exotic states of matter.

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SELF-COMPENSATION AND BONDING-CONVERSION IN B-BASED AND AL-BASED ICOSAHEDRAL CLUSTER SOLIDS

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We have constructed a unified picture for B- and Al-based icosahedral cluster solids [1]. The common features are as below; (1) they should have complicated structures such as giant unit cell crystals or quasicrystals because of inconsistency between the icosahedral symmetry and the periodicity, (2) they can have both metallic and covalent bonds, because B and Al are located at the boundary of bonding in the periodic table, (3) their Fermi level can be located in the deep pseudo-gap or at the high density of states position because of high symmetry of the icosahedron.

The above first feature induces the self-compensation phenomena. The crystalline structure of β -rhombohedral boron (0/1-2/0 approximant) is constructed from the electron deficient B_{12} icosahedra and the electron excess B_{28} clusters, and the former is compensated by the interstitial boron atoms (max 25%) and the latter is compensated by the vacancies at the certain site (also max 25%). When electrons are doped from Li or Mg atoms in the doping sites, first the interstitial boron atoms are removed, and second the vacancies are introduced at the other site, to compensate the electrons [2]. The similar self-compensation phenomena have been reported in the approximant crystals of Al-based icosahedral quasicrystal. In Al-Mn-Fe-Si 1/1-cubic approximants, an increase in the valence electrons due to the replacement of Mn atoms by Fe atoms is compensated by an increase in the number of vacancies in the glue sites [3].

The above second feature induces the metallic-covalent bonding conversion. Both in the B_{12} and Al_{12} icosahedral clusters, the metallic-covalent bonding conversion is occurred whether the center of icosahedron is occupied by the atom or not [4]. This is confirmed experimentally, i.e. the Al_{12} icosahedral cluster with Re center atom in $Al_{12}Re$ 1/0-cubic approximant has metallic bonds and the Al_{12} without the center atom in Al-Re-Si 1/1-cubic one has covalent bonds [5]. The metallic-covalent bonding conversion can occur at the other sites than the center of the icosahedron. When a V atom is doped in the A_1 site of β -rhombohedral boron, the bonding nature is converted from the covalent one to the more metallic one [6].

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ONCE UPON A TIME IN KAMCHATKA:
THE SEARCH FOR NATURAL QUASICRYSTALS

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Twenty-five years ago, soon after the concept of quasicrystals was introduced [1] and the first examples were synthesized in the laboratory [2], the search for a naturally-forming quasicrystal began. For many years, the search was informal. However, beginning about a decade ago, a systematic search [3] was developed that, through planning and much serendipity, led to the discovery this past year of a natural candidate embedded in a rock reported to have been found in a remote region on the northern Kamchatka peninsula [4]. The talk will describe the search for natural quasicrystals and the implications for physics and geology.

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NEW COMPLEXITY IN SELF-ASSEMBLY OF THREE COMPONENT POLYMER MATERIALS

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Block copolymers with incompatible components are known to form periodic structures with mesoscopic length scale reflecting their giant molecular sizes. Their polymer/polymer interfaces are investigated to possess the common feature of constant-mean-curvature(CMC) surfaces, where both domain size and shape are uniquely chosen. How can “CMC-violation” be introduced? This is the principle theme of this presentation.

Polymeric materials naturally have chain length distribution, and it variously affects on their structures and properties. Fortunately, however, if molecular weight distribution index is not so high, block copolymers tend to show very periodic structures with CMC. But when it exceeds a certain critical value, the system turns to have non-CMC surface. Composition distribution is another important issue in block copolymer, and it also affects self-assembly manner considerably. Blending of component homopolymers with parent block copolymer is another way to produce “violation”. Particularly, low molecular weight homopolymers are easy to dissolve in nano-domains of block chains, and hence they can largely effect on polymer/polymer interfacial structure.

A three-branched ABC polymer has an intrinsic feature, whose domain interface does not include any block-block junction points, and it induces two-dimensional periodic Archimedean tiling structures. As an important extended work for ABC star molecules, a quasicrystalline tiling structure with dodecagonal symmetry, whose side length is ca. 50nm, has been observed for ABC/B_h binary blend, where B_h denote a homopolymer of component B.