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16th INTERNATIONAL CONFERENCE on QUASICRYSTALS

ABSTRACT BOOK

THE 16TH

2025 INTERNATIONAL CONFERENCE ON QUASICRYSTALS

22–27 JUNE 2025
NANCY, FRANCE

ORAL COMMUNICATIONS

Quasicrystals from the edge: Extreme environments, impact craters, and the quest in other celestial bodies

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Until 2009, the only known quasicrystals were synthetic, having been formed exclusively in highly controlled laboratory experiments. Plausibly, the only quasicrystals in the Milky Way Galaxy or perhaps even in the Universe, were the ones manufactured by humans, or so it seemed. Then came the report that an icosahedral AlCuFe-quasicrystal had been discovered inside a small rock fragment from a remote stream in far eastern Russia [1]. Later studies proved the rock to be extraterrestrial, a piece of a rare meteorite (known as Khatyrka).
At present, only a few examples of natural quasicrystals have been discovered. Does that mean that these exotic materials must be extremely rare in the Universe?
During this talk, the author will accompany the audience on a cosmic-scale excursion going from shock-wave experiments [2], nuclear tests debris [3] to recently formed fulgurites [4]. Several reasons will be presented indicating that quasicrystals may prove to be among the most ubiquitous minerals found in the Universe [5].
The Author will also show the new directions/outlooks for the quasicrystal research in natural kingdom [6]. Natural quasicrystals are now known to form under extreme conditions of temperature and pressure—precisely the kind of environments generated during high-energy impacts. When an asteroid collides with a planetary surface, the immense heat and shock waves can create exotic materials that would be difficult or impossible to form under normal geological conditions. In impact craters, tiny droplets of rapidly cooled melt could trap quasicrystals, preserving them as microscopic records of these violent events. Similarly, the harsh and unaltered environment of the Moon offers a pristine laboratory for their discovery. Lunar regolith, continuously bombarded by meteoroids for billions of years, may contain quasicrystals formed in extraterrestrial impacts, providing crucial insights into both their natural formation processes and the fundamental physics of matter under extreme conditions.
The discovery of a new quasicrystal (or a new quasicrystal-forming system) in impact crater rocks or on the Moon would be a groundbreaking milestone in our understanding of extreme materials and planetary processes. It would further confirm that nature can forge these exotic structures, expanding our knowledge of high-energy mineral formation and the fundamental principles governing solid matter. Such a find could also offer clues about the early solar system, the impact history of celestial bodies, and even potential materials that might exist on asteroids or other planets. Ultimately, it would push the boundaries of both geology and materials science, opening new frontiers in our search for the most unusual forms of matter in the universe.

Acknowledgements: This study was conducted within the Space It Up project funded by the Italian Space Agency, ASI, and the Ministry of University and Research, MUR, under contract n. 2024-5-E.0-CUP n. I53D24000060005.

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New icosahedral quasicrystals and approximants in Zn-TM-Yb (TM=transition metal)

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Partial substitution of constituent elements in the $Zn_{17}Yb_3$ 1/1 approximants[1] has led to the discovery of new quasicrystals and approximants. To date, quasicrystals have been found in the Zn-Mg-Yb [2] and Zn-Au-Yb [3] systems, while 2/1 approximant in the Zn-Au-Yb system and 1/1 approximants in the Zn-Au-Yb [3], Zn-Al-Yb [1], and Zn-Cu-Yb [4] systems. However, systematic studies on elemental substitution in $Zn_{17}Yb_3$ 1/1 approximants[1] remain limited to the above alloy systems.

In this study, we explored new quasicrystals and approximants in the Zn-TM-Yb (TM = transition metal) systems by substituting Zn with TM in the $Zn_{17}Yb_3$ 1/1 approximants with 11 TMs (V, Cr, Mn, Fe, Co, Ni, Zr, Nb, Pd, Ag, Pt). As a result, we found an icosahedral quasicrystal and a 2/1 approximant in the Zn-Pt-Yb system, and 1/1 approximants in the Zn-(Ag, Mn, Fe, Cr, Pd, Pt) -Yb systems. We investigated the formation of the Zn-Pt-Yb icosahedral quasicrystal and 2/1 and 1/1 approximants in detail. The single phase of Zn-Pt-Yb quasicrystal was obtained in an alloy slowly cooled from the melt at a rate of -15 K/h and alloys annealed at different temperatures (673-983K) for 100 hours. Thus, the icosahedral quasicrystal is thermodynamically stable, in contrast to the metastable Zn-(Au, Mg)-Yb quasicrystals. In this presentation, we will also present the results of magnetic susceptibility measurements and crystal structure analysis of the approximants.

Acknowledgements: This research was supported by JSPS Grant-in-Aid for Scientific Research 24K08041.

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A new *oF*-type elemental boron phase synthesized by the rapid quenching -Search for semiconducting quasicrystal-

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We have previously reported by first-principles calculations that pure boron can have β-rhombohedral-type 1/1-cubic approximants and β-rhombohedral-type quasicrystals as metastable phases. [1] We therefore searched for quasicrystals by quenching a supercooled liquid of pure boron.

Several phases of boron are known, consisting of icosahedral clusters of boron (B_{12}). Recently, a structural model for τ-orthorhombic boron [2] has been proposed based on the atomic arrangement of β-rhombohedral boron (B_{105}) (space group R-3m with a = 10.139 Å and α = 65.199° cell) [3]. τ-orthorhombic boron belongs to the orthorhombic crystal system (space group: Cmcm) with lattice parameters a = 10.923 Å, b = 17.003 Å, and c = 17.562 Å. While α- and β-rhombohedral boron are considered to be 0/1-2/0 rhombohedral approximants, τ-orthorhombic boron is believed to be a 1/0-1/0-0/1 orthorhombic approximant, which is a higher approximant (unit cell volume four times larger) and is the same as the carbon-trace metastable phase derived from α-rhombohedral boron [4].

We have quenched electrostatically levitated supercooled liquid boron [5] by the Hammer quench method. As a result, in addition to the stable β-rhombohedral boron phase, the metastable α-tetragonal boron phase and an unknown phase were obtained. Three-dimensional electron diffraction tomography of the quenched sample revealed a new orthorhombic face-centered (oF) structure with a unit cell of a = 30.97(7) Å, b = 10.83(11) Å, and c = 17.18(6) Å. This new phase is thought to have a structure with twice the lattice constant in the c-axis direction of τ-orthorhombic boron (and twice the unit cell volume), and the structural model was in good agreement with the ABF and HAADF images obtained by atomic resolution STEM. In addition, in samples with different quenching rates, the volume fraction of the new oF phase increased with increasing quenching rate, similar to the metastable α- tetragonal boron phase. This suggests that the new oF phase is also a metastable phase and was not generated by the incorporation of carbon, as in the case of τ-orthorhombic boron.

Acknowledgements: This study was partly supported by JSPS KAKENHI grant numbers JP19H05818, JP19K05643, JP20H05258, JP20H00189, JP23K04373, JP23K26367 and as well as by the GIMRT program (Nos. 202211-RDKGE-0008 and 202311-RDKGE-0001) at the Institute for Materials Research, Tohoku University.

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Theoretical analysis of Tsai-like and Bergman-like models of 1/1 ZnMgHf periodic approximant crystal

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The great investigation opportunity of the similarity between Tsai and Bergman-type phases come with the Zn-Mg-(Hf, Zr, Ti) system. In the system, Bergman F-phase is right next to the Tsai P-phase quasicrystal in the composition phase diagram. Also, there is 1/1 cubic approximant crystallizing in $Im\bar{3}$ space group modelled by Gómez, et al. [1]. The model puts partially occupied atoms in the sites forming triangle of two soccerball polyhedron vertices and one site that should be unoccupied in ideal Bergman-type phase. The site however should be occupied in Tsai-type phase [2].
Calculations were performed with Quantum Espresso suite of program in version 6.7 [3, 4] with PBE pseudopotential for Zn-Mg-Hf. DFT+U was used but changes to electronic structure are marginal in comparison to calculation without Hubbard correction.
The energy difference between Bergmam-like and Tsai-like model differs by only 10 meV in favour of Tsai-like model. Calculated Madelung energy based on Löwdin charges correlates with total energy trend. The Tsai-like model exhibits increased peak in the pseudogap region of the density of states. High density of states at the Fermi level correlates with low resistivity measured with four point method on quasicrystalline sample. Comparatively to Al-Cu-Fe Mackay quasicrystal, which has $\rho_0 = 10\,000\ \mu\Omega \cdot \mathrm{cm}$, Zn-Mg-Hf has $\rho_0 = 48\ \mu\Omega \cdot \mathrm{cm}$. The analysis of the Electron Localization Function and Maximally Localized Wannier Functions indicates presence of three-center bonds (Fig. 1.). Bonds centers are also found in tetrahedral positions.

Fig. 1. The local environments of Wannier centers around Zn14 atoms (additional for the Bergman-like model). Three center bonds (green) are visible with accompanying two-center (ligh-blue). Atom labels as in [1].

Acknowledgements: We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017147. This work was supported by the National Science Centre Poland, grant no. UMO-2022/47/I/ST3/00340

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Quasicrystal stability and nucleation kinetics from density functional theory

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Are quasicrystals stable or metastable? Density functional theory (DFT) is often used to evaluate thermodynamic stability, but quasicrystals are long-range aperiodic and their energies cannot be calculated using conventional *ab initio* methods. Here, we perform first-principles calculations on quasicrystal nanoparticles of increasing sizes, from which we can directly extrapolate their bulk and surface energies. Using this technique, we determine with high confidence that the icosahedral quasicrystals $ScZn_{7.33}$ and $YbCd_{5.7}$ are ground-state phases—revealing that translational symmetry is not a necessary condition for the $T = 0$ K stability of inorganic solids. Although we find the $ScZn_{7.33}$ quasicrystal to be thermodynamically stable, we show on a mixed thermodynamic and kinetic phase diagram that its solidification from the melt is nucleation-limited, which illustrates why even stable materials may be kinetically challenging to grow. Our techniques here broadly open the door to first-principles investigations into the *structure-bonding-stability* relationships of aperiodic materials.

[1] *Nature Physics* (2025, *in press*)

Structural Stability and Transport Properties of TiZrNi Quasicrystals under High Pressure

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We report on the structural and transport properties—including superconductivity, resistivity, and magnetization—of $Ti_{53}Zr_{27}Ni_{20}$ quasicrystals under high pressure, studied using a diamond anvil cell. These properties are also compared with those of hydrogenated samples. The superconducting transition temperature (Tc) of the pristine powder was found to be 1.94 K at 0.78 GPa, increasing steadily to 6.47 K at 75 GPa. Similarly, the hydrogenated samples exhibited an increase in Tc with pressure, albeit with an approximate delay of 0.8 K relative to the pristine samples. Synchrotron-based X-ray diffraction revealed that $Ti_{53}Zr_{27}Ni_{20}$ quasicrystals absorbed 3.4 wt.% hydrogen at 5.08 GPa without undergoing a phase transformation. Approximately half of the absorbed hydrogen was released upon pressure reduction, indicating the potential utility of TiZrNi quasicrystals in practical hydrogen storage applications. Interestingly, the 1/1 approximant phase of TiZrNi was observed to transform into a quasicrystalline phase upon decompression from pressures above approximately 20 GPa. The high-pressure dynamics and structural stability of TiZrNi quasicrystals will be discussed.

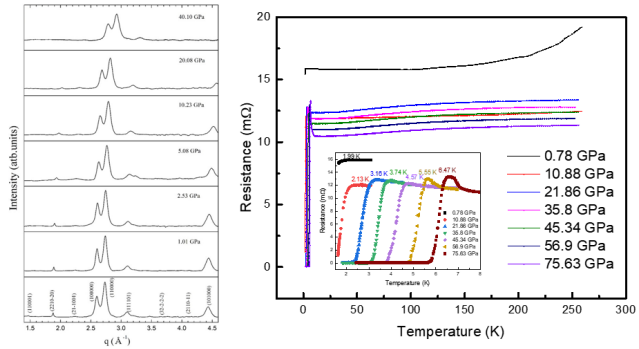

Fig.1: The synchrotron-based XRD (left) and resistance data (right) of $Ti_{53}Zr_{23}Ni_{20}$ quasicrystals at high pressure.

Phason relaxation in the Spectre tiling

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The recently discovered Spectre tilings [1] are quasiperiodic [2]. A physical realization of a density corresponding to a decoration of the Spectre prototile therefore possess symmetries associated with the relative phases of incommensurate density waves, and the spontaneous formation of such a structure would require the relaxation of phason deformations associated with long wavelength variations in these relative phases. In the context of a tiling model, the relaxation process must proceed via a sequence of local rearrangements of the tiles.

In the familiar cases of quasicrystalline tilings consisting of rhombic (or rhombohedral) prototiles, phason rearrangements can be modeled as flips of local clusters that have the effect of moving a mismatch in the tiling along a linear (or planar) structure known as a worm. For the Spectre tiling, the analogous rearrangements of tiles and the structure of worms are more complex, and there is no obvious way to formulate a model that allows for the simulation of phason relaxation using the Spectre tiles themselves. I will describe the structure of phason displacements in the Spectre tiling, present a model that allows for simulation of phason relaxation through local rearrangements, and present results on the dynamics of the relaxation process.

Acknowledgements: I thank P. Mostert for helpful exchanges within tiling@googlegoups.com.

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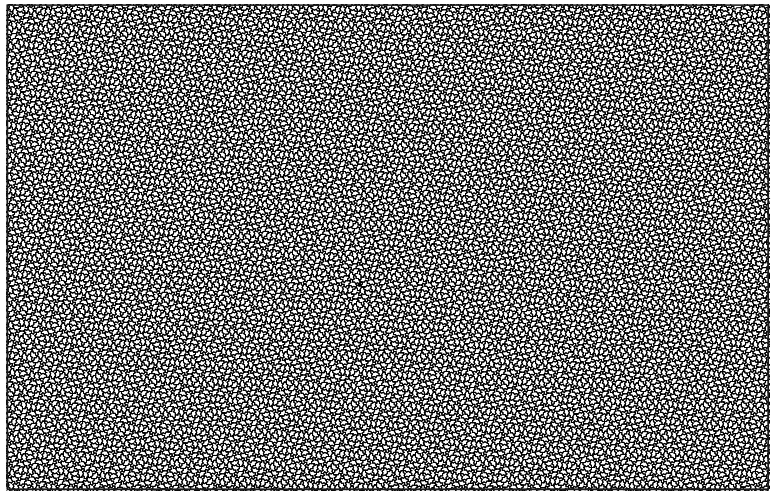

Fig 1. A portion of a Spectre tiling highlighting a network of worms associated with phason shifts.

Aperiodic tilings for relating crystals, quasicrystals and modulated structures

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Aperiodic crystals constitute a class of materials that includes quasicrystals and modulated structures. A key challenge in this field is understanding the similarities and differences between periodic and aperiodic crystalline structures. To address this issue, we investigate the relationship between crystals, quasicrystals, and modulated structures.

First, we propose aperiodic tilings composed of large and small hexagons, and parallelograms, as shown in Fig. 1(a). These tilings have self-similar structures characterized by metallic mean $\tau_k = (\sqrt{k^2+4}+k)/2, (k = 1, 2 \ldots)$. One of the important properties is that the tilings serve as aperiodic approximants for the honeycomb lattice: as the metallic mean increases, the size of honeycomb domains bounded by the parallelograms also increases, and the whole tiling converges to the honeycomb lattice. This suggests that the tilings have not only quasicrystal but also modulated structures. Furthermore, we demonstrate that the superspace structural analysis on the tilings can be applied to a soft-matter system exhibiting modulated structures. These results clarify that crystals, quasicrystals and modulated structures are bridged through superspace analysis [1].

We also present a method for generating hexagonal aperiodic tilings that are topologically equivalent to the triangular and dice lattices. This approach incorporates aperiodic sequences into the spacing between three sets of grids for the triangular lattice, resulting in "modulated triangular lattices", as shown in Fig. 1(b). Subsequently, by replacing the triangles with rhombuses and parallelograms, a modulated dice lattice is constructed. These lattices can be regarded as the continuous modulation of the periodic lattice. Furthermore, by using the generalized Fibonacci, Thue-Morse, and tribonacci sequences, we demonstrate several examples of hexagonal aperiodic tilings. Our method establishes a general framework for constructing a broad range of hexagonal aperiodic systems, advancing aperiodic-crystal research into higher dimensions that were previously focused on one-dimensional aperiodic sequences [2].

Acknowledgements: T.M. was supported by International Exchange Grant from Tateisi Science and Technology Foundation, and JST SPRING, Japan Grants Nos. JPMJSP2106 and JPMJSP2180. This work was also supported by Grant-in-Aid for Scientific Research from JSPS, KAKENHI Grant Nos. JP22K03525, JP21H01025, JP19H05821 (A.K.) and JP24K06982 (T.D.).

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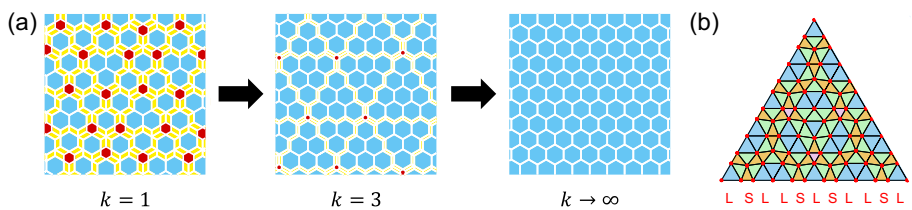

Fig.1: (a) Metallic-mean tilings serving aperiodic approximants of the honeycomb lattice. (b) Triangular lattice modulated by the Fibonacci sequence.

Zero-temperature structure of icosahedral quasicrystals: density-functional scrutiny

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We scrutinize current understanding of atomic structures of all families of intermetallic icosahedral quasicrystals by zero-temperature density-functional evaluation of their energetic stability. In order to faithfully represent quasicrystal structure, the simulations are performed in « sufficiently large » periodic approximants tiled by *all four* cells of the Canonical Cell Tiling (CCT), even though the structures we obtain from simulations are not necessarily CCT decorations. This approach warrants that we represent all atomic motifs that are necessary to build infinite quasicrystal (QC).

Our study encompasses the so called Frank-Kasper i-QC family (AlMgZn, AlCuLi, MgZnY), pseudo-Mackay family (AlMnPd, AlCuFe, AlCuRu), as well as Tsai-QC family (ZnSc, ZnMgSc, CdYb). We also discuss phases that appear to be intermediate between Frank-Kasper and Tsai classes (HfMgZn, MgZnY). Our results are not merely energetic data exposing quasicrystal energies to the competition of the crystalline phases, we also ask, if the energetically optimized QC structures can be faithfully represented by abstract, deterministic models.

Theoretical insights into ultrathin oxide films on metals and alloys: unraveling structures and stabilities

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Thin perovskite films, made of a few-layer thick nano-sheets, have attracted considerable attention due to their extensive structural and electronic variability, linked to the huge number of conceivable unique chemical compositions. The combination of the low dimension with the structural flexibility of this class of crystals opened the door to a rich spectrum of applications in many fields, such as energy transition and catalysis, correlated materials and electronic devices.

Decreasing the thickness of two-dimensional (2D) perovskites down to the mono-layer limit is expected to deeply alter their structures and modify the physical and chemical properties. This has recently led to the emergence of novel structures with aperiodic ordering, i.e. dodecagonal oxide quasicrystal interfaces (Fig. 1) [1,2]. The driving force for these unique structural modifications, resulting from thickness reduction, are far from being fully unveiled [3]. Reduced bonding chemical coordination, possible strong surface polarization, support effect and experimental condition are supposed to play a role, but no clear picture has yet been drawn. This work shows how two-dimensional complex oxide structures can be identified, while also questioning several descriptors that contribute to their stability. It is a first step towards establishing structure-property relationships for this class of materials, which is crucial not only for advancing fundamental understanding of their unique characteristics but also for optimizing their performance in practical applications.

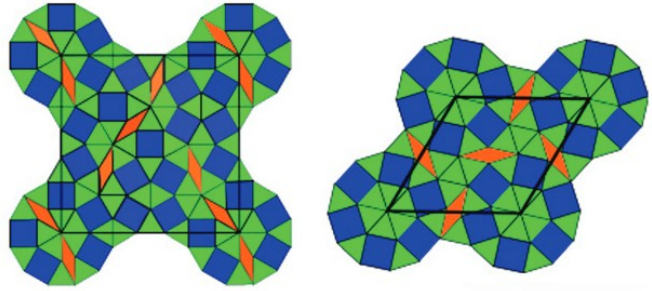

Fig. 1 : Tilings made with square, triangle and rhombus tiles sharing a common edge length (6.7 Å) used to describe the 2D oxide quasicrystalline approximants synthesized in ref. [1]

Acknowledgements: The computational resources (GENCI, TGCC, CINED, IDRIS, EXPLOR) and financial support (ANR NOUS) that made this work possible are aknowledged.

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Hyperuniform properties of the square-triangle tilings

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The structural properties of two-dimensional tiling composed of squares and triangles have attracted significant attention. Periodic and quasiperiodic tiling patterns have been observed in systems such as inorganic materials, liquid crystals, and soft materials. Additionally, aperiodic square-triangle tiling [1], where squares and triangles are distributed aperiodically, has been identified in Mn-Cr-Ni-Si alloys, mesoporous silica, and multicomponent block polymer systems. Unlike previously known periodic and quasiperiodic tiling, square-triangle tiling allows an infinite number of configurations of square and triangle arrangements. Therefore, a systematic characterization of its structural properties is needed.

In this study, we systematically analyze hyperuniform properties of square-triangle tiling [2]. The tiling is constructed based on local growth rules. By introducing a probability p into the growth rules, various square-triangle tiling configurations can be generated. When $p<0.5$, square lattice regions and triangular lattice regions phase-separate, and the variance in point distribution follows a scaling law with an exponent $\alpha<0$. This configuration is classified as anti-hyperuniform. On the other hand, for $p>0.5$, squares and triangles become homogeneously mixed, and the point distribution belongs to hyperuniform class III. These findings suggest the existence of a hyperuniform–anti-hyperuniform transition at $p=0.5$. Furthermore, analysis of the structure factor of square-triangle tiling reveals that the peak structure in the high-wavenumber region is common to almost all tiling configurations, while the peak structure in the low-wavenumber region strongly depends on the hyperuniformity of the tiling.

Acknowledgements: This work was supported by Grant-in-Aid for Scientific Research from JSPS, KAKENHI Grant No. JP22K03525 (A.K.).

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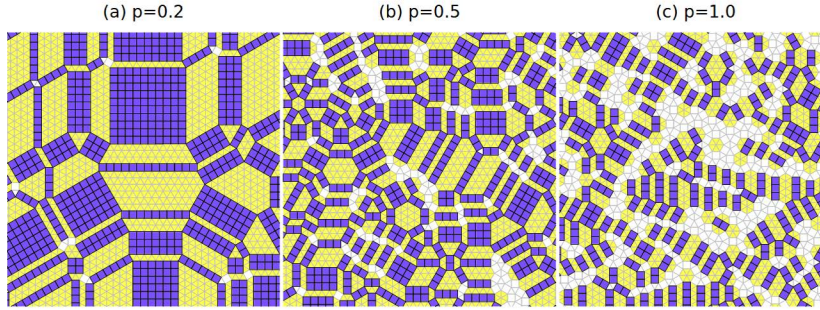

Fig.1: Square-triangle tilings generated by means of the growth rule.

Structure of the hexagon clusters in the Smith et al. Spectre tilings

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Decorating the Spectre aperiodic monotile from *A chiral aperiodic monotile* [1] with a hexagon and a 30 degree rhomb leads to interesting graphs where the hexagons necessarily group in small triangular clusters, which gives an alternative description [2] of the hierarchical structure of Spectre tilings, dual to the one given in [1].

Acknowledgements: Author participation to the conference is paid by ANR project TiGeRS.

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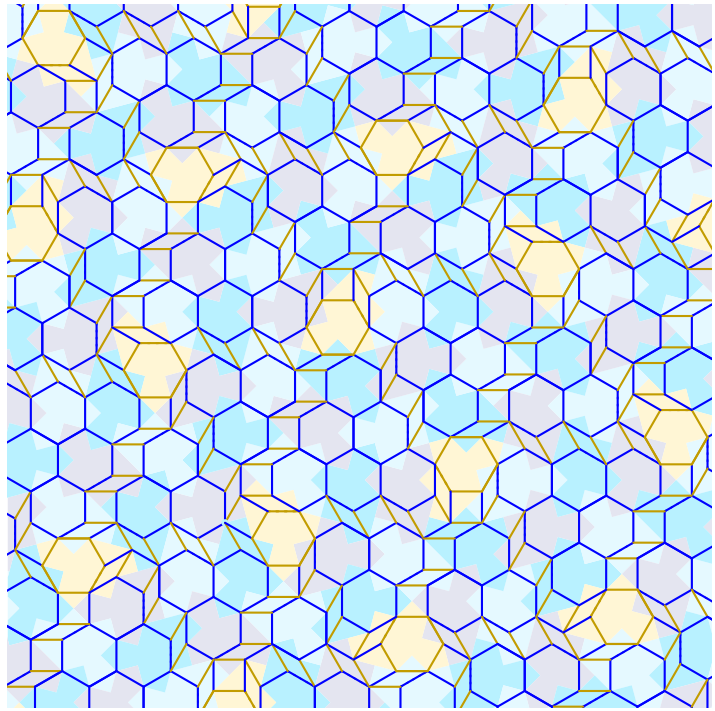

Fig.1: Decorated Spectre tiling

On the long-range order of the Spectre family of tilings

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In 2023, J. Smith et al. presented two aperiodic tilings of the plane, the Hat [1] and the Spectre [2] tilings, each of which consisted of rotated and (in the Hat case) reflected copies of a single polygonal prototile, and whose aperiodicity is enforced alone by the geometric matching conditions of the tiles. These aperiodic *monotile* tilings immediately attracted considerable attention. Each of them is in fact part of a continuous family of tilings with similar properties.

The detailed structure of the Hat family of tilings had been analysed in [3]. The key was the existence of a self-similar member of the Hat family, called the *CAP tiling*, for which we could prove that it is a cut-and-project set (CPS) with pure-point diffraction. Due to the simple topology of the CAP tiling, all the other family members are then mutually locally derivable (MLD) with deformed versions of the CAP tiling, and have pure-point diffraction, too, with the same set of Bragg points. In fact, up to rotation and scale, all Hat family tilings are MLD with point sets obtained from the same CPS as the CAP, but with projections in different directions.

Here, we present a similar analysis [4] for the Spectre tilings. Roughly speaking, everything is a bit more complicated, but qualitatively quite similar to the Hat tilings. Also here, we determine a geometrically self-similar member of Spectre family, which we call the CASPr tiling, and which we show to be a CPS with pure-point diffraction. Its inflation is a bit special, in that it maps tiles to scaled, rotated, and *reflected* supertiles, which are the replaced by patches of the original tiles. Starting from the CASPr, all other members of the family are then MLD to deformed CASPr tilings, and due to the simple topological nature of the CASPr, all these deformed tilings are, up to rotation and scale, topologically conjugate to the CASPr, and hence share the same diffraction spectrum. In fact, we have again a vast family of tilings whose structures are all closely related. Up to scale and rotation, they are MLD to point sets obtained from a single CPS, but with different projection directions.

This analysis paves the ground for the actual computation [4] of the diffraction patterns of the different Spectre family tilings, which will be presented by Jan Mazáč at this conference.

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Homochiral inflation for the aperiodic monotile Tile(1,1)

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The recently discovered chiral monotile Tile(1,1) [1] is tiling the plane in a quasiperiodic fashion by taking twelve different orientations when applying $2\pi/12$ rotation. An homochiral inflation construction of such a quasiperiodic tiling is proposed [2] where the chirality of the monotile is completely fixed at all inflation steps, avoiding to exchange its chirality between two successive steps. Doing so, the twelve possible orientations of the monotile are explicitly coded and the key difference between odd and even orientations is considered. The tiling is decomposed using only two different clusters, Γ and Ω, each of them taking six possible orientations. This gives a total set of twelve metatiles, which assembly can be mapped onto a triangular lattice.

This approach allows to properly separate rotation and translation symmetry elements relating monotiles together. As all possible orientations of the two clusters are already incorporated in the twelve metatiles, positions of adjacent metatiles are given by translations which are along three equivalent directions ($2\pi/3$ rotation) as evidenced by junction lines. Finally, thanks to the homochiral inflation, the orientation distribution of the monotile at each inflation step is computed.

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Phason modes in icosahedral quasicrystals

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Phason modes in quasicrystals have been evidenced experimentally by X-ray or neutron diffuse scattering measurements [1]. For a better understanding of phason modes, realistic atomic modeling is necessary. In the first part of the presentation, we discuss six-dimensional models of icosahedral quasicrystals in terms of local reorganization of the cluster arrangements [2]. In the second part, we discuss the phason modes studied by high-resolution X-ray diffraction and absolute scale diffuse scattering measurement [3, 4].

Acknowledgements: This research was supported by JSPS Grant-in-Aid for Scientific Research 24K08041.

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The phonons of oxide quasicrystals by surface-sensitive inelastic electron scattering

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Twelve years ago, oxide quasicrystals have been discovered [1]. Dodecagonal oxide quasicrystals (OQC) are two-dimensional structures with long-range order, sharp twelve-fold diffraction pattern and well-defined self-similar tiling pattern. Examples are Ba-, Sr-, or Eu-decorated $Ti_2O_{3+\delta}$ planar networks on the surface of close-packed metals such as Pt(111) or Pd(111). The OQC formation leads to self-similar but aperiodic triangle-square-rhomb tiling structures, which were proposed as purely mathematical concepts decades ago [2]. Depending on the preparation conditions, such aperiodic structures can coexist with *periodic* triangle-square-rhomb tilings known as quasicrystalline approximants [3,4].

Here we present surface-sensitive vibrational spectroscopy data for two different OQCs, the cases of the Ba-Ti-O quasicrystal on Pt(111) and of the Eu-Ti-O quasicrystal on Pd(111), together with their low-energy electron diffraction (LEED) patterns. Although both two-dimensional layers have aperiodic dodecagonal structures, they exhibit clear dipole-active surface phonons in high-resolution electron energy loss spectroscopy (HREELS). The HREELS spectra are dominated by two strong phonon modes at 595 and at 71 cm^{-1} for Ba-Ti-O (Fig. 1), as well as at 569 and 67 cm^{-1} for Eu-Ti-O. The low-energy modes at 71 and 67 cm^{-1} are assigned to the out-of-plane vibrations of the Ba and the Eu atoms, respectively. Vibrational spectra for the planar binary Ti_2O_3 honeycomb network on Pt(111), on the other hand, identify the phonon modes around 550 cm-1 to the phonons of the planar Ti-O-Ti bonds. These bonds are shifted in both OQCs due to the modifications of the Ti-O-network and due to the Ba- or Eu-decoration of the network pores [5].

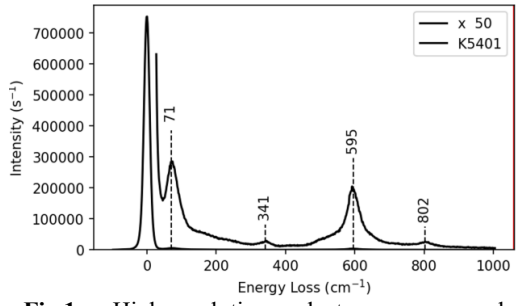

Fig.1: High-resolution electron energy loss spectrum of a dodecagonal Ba-Ti-O quasicrystal on Pt(111).

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Ab initio calculations of magnetism in Cd_6Tb 1/1 periodic approximant of a Tsai-type quasicrystal

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From the beginning of the discovery of quasiperiodicity in intermetallic compounds magnetic properties were in the center of interests. The possibility of exotic behaviour due to intrinsic quasiperiodicity was high. The magnetic structure was investigated in numerous phases bearing Rare-Earth elements as possessing localized magnetic moments. The first long-range magnetic order was discovered in Im-3 Cd_6Tb 1/1 cubic approximant crystal [1]. Tb atoms are grouped in icosahedral shell of Tsai-type rhombictriacontahedral clusters being structural units. The orientation of magnetic moments for vertex- and body-centered clusters is antiparallel constituting antiferromagnetism. The transition temperature is 24 K with effective magnetic moment equal to 9.8 μ_B. The aim of the study is to deliver the theoretical justification on the existence of long-range magnetic order in Cd_6Tb based on the electronic structure calculations.

Density functional theory calculations were performed using Quantum Espresso [2,3]. PBE exchange correlation functional was chosen with PAW pseudopotentials. Energy cutoffs for wavefunctions and charge density were set to 125 Ry and 625 Ry, respectively. Selfconsistent calculations were done in Γ point only and density of states on a 4^3 k-point grid.

Tb-4f electrons form atomic-like states near the Fermi energy which slow the convergence and require large energy cutoffs. Firstly, we considered the experimental crystal structure. Scalar-relativistic calculations fail to predict the correct ground state because ferromagnetic configuration is slightly favoured by 0.1meV/atom and the magnetic moments equal 6.0 μ_B per Tb atom are too small. Nonmagnetic structure has higher total energy by 55 meV/atom. The Fermi surface is built mainly from Tb-4f states with small contributions from Tb-5d and Cd-5p. DFT+U calculations using Cococcioni's simplified approach [4] with single parameter U = 8 eV increased the magnetic moments by 0.4 μ_B. The inclusion of the spin-orbit coupling favours antiferromagnetic configuration with a large energy difference of over 300 meV/atom against the ferromagnetic one. Magnetic moments converged slowly to approximately 8.2 μ_B. Then we used the cell with relaxed volume and fixed experimental atomic positions. The lattice constant increased by 0.9 a_B and the magnetic moments converged to 9,2 μ_B. Atomic position relaxation was omitted because of large computational time. Overall, our calculation indicate the importance of the spin-orbit coupling and volume relaxation in the confirmation of the antiferromagnetism in the Cd_6Tb cubic approximant.

Acknowledgements: This work was supported by the National Science Centre Poland, grant no. UMO-2022/47/I/ST3/00340 and by Polish high-performance computing infrastructure PLGrid (Cyfronet AGH) grant no. PLG/2024/017306.

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Accelerating quasicrystal discovery with machine learning

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Discovering novel quasicrystals (QCs) traditionally relies on serendipity or extensive, often slow and costly, experimental searches. Machine learning (ML) offers a powerful data-driven alternative to accelerate this process. By learning complex composition-structure relationships from existing data [1, 5], ML models can efficiently screen vast chemical spaces and guide experimental synthesis towards promising QC candidates.

Our recent efforts have focused on developing and applying ML methodologies to the challenge of quasicrystal prediction and discovery. We initially developed ML models capable of predicting the likelihood of QC formation solely based on chemical compositions, leveraging carefully curated datasets [1, 5]. This approach successfully predicted several new QCs, which were subsequently confirmed through experimental synthesis and characterization [3]. Furthermore, we have employed deep learning techniques for the rapid identification of new QCs directly from multiphase powder X-ray diffraction patterns, demonstrating the potential for automated phase analysis in complex systems [2]. Foundational to these efforts is the compilation of comprehensive experimental datasets encompassing known QCs and their approximants, which serve as crucial training grounds for robust ML models [5].

Looking ahead, our future work aims to discover QCs with specific, targeted functionalities. We plan to integrate advanced structure prediction with functional output regression techniques [4] to predict not only phase stability but also key physical properties like electronic band structures. A particular focus is the discovery of novel semiconductor QCs, exploring their unique properties for potential electronic applications.

Acknowledgements: This work was supported by the Grants-in-Aid for Scientific Research on Innovative Areas (19H05817, 19H05818, 19H05820), and the JST-CREST project (JPMJCR22O3).

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Fingerprinting Phason Strain Using Diffuse Multiple Scattering

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Diffuse Multiple Scattering (DMS) [1-3] occurs in single crystals when an elastic internal divergent source of X-rays is subsequently scattered by diffracting planes. This source is provided by the diffuse scatter arising from a disruption in the long-range order of the crystal such as structural defects or crystal-surface truncation. DMS manifests as diffraction lines similar to Kossel lines which, unlike DMS lines, arise due to fluorescence. The elastic nature of DMS lines means that multiple line intersections can be forced using synchrotron radiation by changing the incident energy [2]. Because multiple projections are collected simultaneously without moving the sample, the technique offers high precision and flexibility in terms of crystal orientation and in situ experiments in the presence of various external stimuli [2-3].

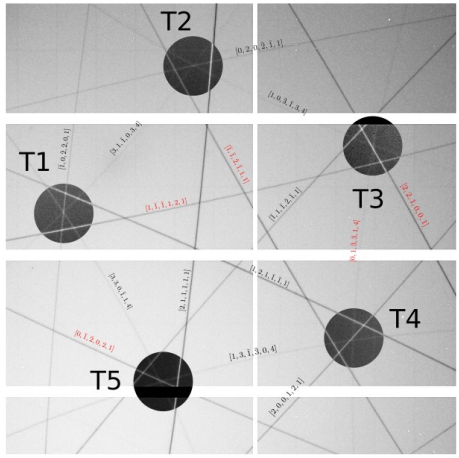

Figure 1: DMS pattern of an icosahedral quasicrystal along the 5-fold axis.

The DMS pattern of the icosahedral quasicrystal is indexed using a 6 dimensional cubic reciprocal lattice (6 integer indices). The 6D reciprocal vector is expressed as the sum of the physical space component (3D) and the so-called perpendicular or phason component (3D). Any departure from the perfect icosahedral symmetry can be expressed in term of a strain of the 6D lattice along the 'phason' component, using the so-called phason strain matrix [4].

By selecting a scattering geometry such that the 5-fold axis is perpendicular to the incident beam and parallel to the detector normal, a 5-fold pattern is observed. By selecting an appropriate wavelength, 5 equivalent triple line intersections can be observed simultaneously. However, a departure from the icosahedral symmetry results in some of the intersections being split, providing a binary fingerprint for the presence of phason strain. Furthermore, precise determination of the phason strain can be achieved by fitting the DMS lines which only requires a few minutes of data collection. I will present analysis from i-AlCuRu and i-AlPdMn quasicrystals.

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Phys. Rev. Materials **5**, L120601 (2021)
A. G. A. Nisbet, M. G. Cain, T. Hase and P. Finkel
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J. App. Cryst. 56 4 2023
A. G. A. Nisbet, M. G. Cain, T. Hase and P. Finkel
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Oxford University press, 2018
Ted Janssen et al.

Monstrous Covariograms of Rauzy Fractals

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For one-dimensional model sets, which form a mathematical model for quasicrystals, the averaged distance structure is determined via its *pair correlation function*. This function simply describes, on average, how often one finds two points of the model set at a given distance. Moreover, there is a natural representation via the *covariogram of the window.* While they can be simple tent-shaped functions for interval windows, the more typical case of inflation systems with *Rauzy fractals* exhibit complex and unexpected behaviour. We give a concrete example and use a renormalisation procedure on the pair correlation functions to exactly calculate the resultant monstrous covariogram.

Acknowledgements: This work was supported by the German Research Foundation (DFG, Deutsche Forschungsgemeinschaft) via Project A1 within the CRC TRR 358/1 (2023) – 491392403 (Bielefeld – Paderborn).

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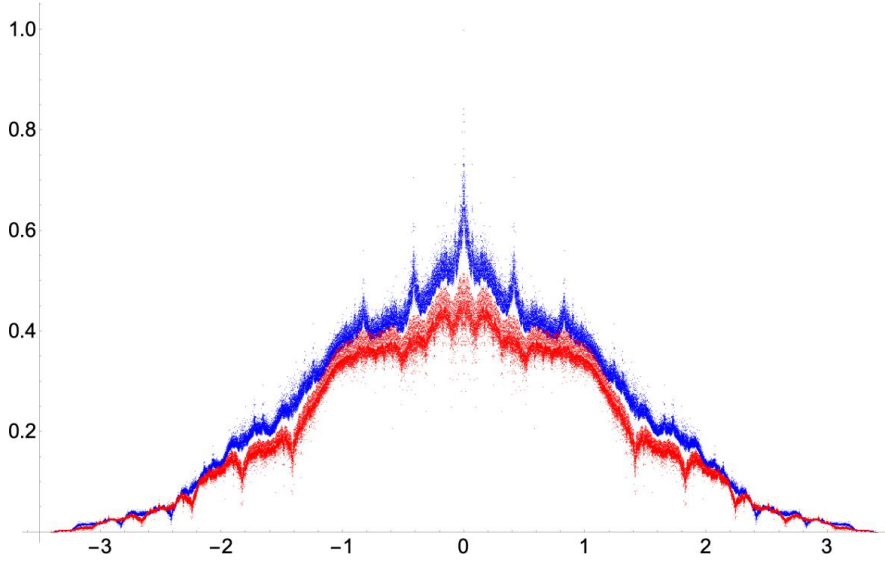

Fig.1: Point plot, with 188214 points, of the covariogram of the window corresponding to the inflation $a \to aaaaabb,\ b \to baa.$ The splitting behaviour is highlighted, with the distances possessing an even number of b's are blue, and those with an odd number are red.

Octagonal tilings with three prototiles: part 1

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Motivated by theoretically and experimentally observed structural phases with octagonal symmetry [1,2], we introduce a family of octagonal tilings which are composed of three prototiles [3].

In the first part of our talk, I will discuss our motivation and differing approaches to solving the same problem. Then, I will introduce the tilings, which are composed of three prototiles: a small square T_1, an isosceles triangle T_2, and a large square T_3. I will show that the tiling family can be defined with respect to two non-negative integers *m* and *n*, such that the inflation factor of a given tiling is $\delta_{(m,n)} = m + n(1 + \sqrt{2})$. From here, I will demonstrate how our infinite series of tilings can be delineated into separate cases, determined by the relationship between *m* and *n*.

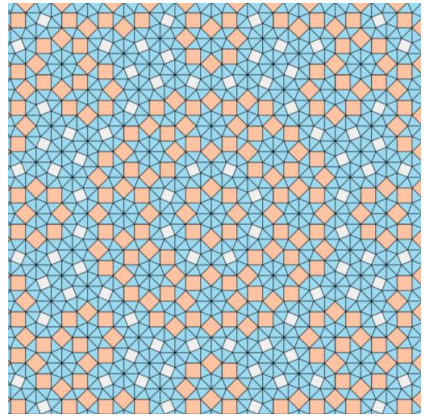

Fig.1: A patch of the m=n=1 tiling.

Acknowledgements: The authors express their gratitude to Marianne Impéror-Clerc, Frank Smallenburg and Andrea Plati for helpful discussions. SC acknowledges that this work was supported by EPSRC grant EP/X011984/1, while ALDS is grateful to De La Salle University for the conference grant provided through the Faculty Development Program.

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Octagonal tilings with three prototiles: part 2

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In the second part of our talk, I will discuss some statistical properties of our tilings, including the area fractions of the prototiles and patch frequencies. These properties are derived from a general substitution matrix [1], which counts the occurrences of each prototile within $\delta_{(m,n)}T_i$, $i = 1, 2, 3$. The matrix is given by:

$$M_{(m,n)} = \begin{bmatrix} m^2+n^2 & \frac{mn}{2}+b & 0 \\ 8mn+8n^2 & m^2+4mn+3n^2+4b & 8mn+8n^2 \\ 0 & n^2-2b & m^2+2mn+3n^2 \end{bmatrix},$$

where $b = 0$ for $m \geq n$ and $b = \frac{(n-m)^2}{4}$ for $0 \leq m < n$.

I will then compare our family of tilings with existing examples in the literature. Specifically, I will compare the area fractions of the prototiles with those in the QC8 tilings [2]. Following that, I will discuss a local replacement rule that transforms one of our tilings into a new tiling composed of rhombs and squares. This new tiling is closely related to both the Ammann–Beenker tiling [3, 4] and the Watanabe–Ito–Soma tiling [5].

Acknowledgements: The authors express their gratitude to Marianne Impéror-Clerc, Frank Smallenburg and Andrea Plati for helpful discussions. SC acknowledges that this work was supported by EPSRC grant EP/X011984/1, while ALDS is grateful to De La Salle University for the conference grant provided through the Faculty Development Program.

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The three-colour problem in quasiperiodic tilings

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Singh *et al.* [1] discussed in a recent paper the colouring of the Ammann-Beenker tiling with three colours. Colouring with three colours (3-colouring) implies that tiles with equal colour do not have contact at edges whereas contact at vertices is possible. Due to stimulation by this paper, several quasiperiodic tilings with different rotational symmetries and other symmetries [2] were 3-coloured. The result was that a large amount of quasiperiodic tilings can be 3-coloured. According to [1] the 3-colouring of Penrose rhomb pattern was described in [3]. Tilings composed of rhombi can be 3-coloured. Rules were searched which enable or prohibit the decoration with three colours. For this reason, the 3-colouring of so-called p^q-tilings (q p-gons sharing a vertex) was considered. p^q-tilings exist in spherical, Euclidean and hyperbolic space. With p = odd and q=3 the decoration with three colours is ruled out. This result holds for quasiperiodic tilings analogously. 'Dead surfaces' and 'forced colours' were also used to derive the exclusion of 3-colouring. The decoration within the dead surface is unique.

One should keep in mind that 3-colouring does not imply that there is any colour symmetry. Quasiperiodic tilings with colour symmetry and three colours are very scarce. Nevertheless, some of the decorations exhibit special colour symmetries.

The possibility of a colour flip was detected for some decorated tilings. If a closed loop formed by one of the three colours exists within the tiling, the two other colours may interchange within the area surrounded by the loop. A colour flip destroys colour symmetries.

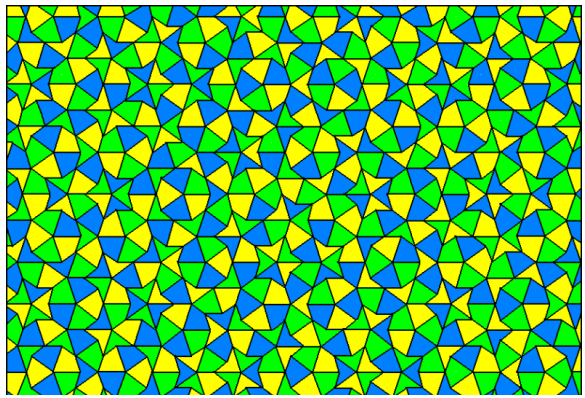

Fig. 1: Decoration with three colours of Penrose's kite and dart pattern.

Numerical methods for quasiperiodic systems

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Quasiperiodic systems, inherently linked to irrational numbers, are significant space-filling constructs that lack decay and translational invariance. Nevertheless, due to the computational challenge of storing and representing irrational numbers in computers, Diophantine errors—arising from the approximation of irrational numbers by rational ones—inevitably occur during numerical computations of quasiperiodic systems, where irrational numbers are fundamental. These errors can critically affect the accuracy of calculation outcomes. This talk will dissect the mechanism of Diophantine errors and their ramifications on numerical computations. It will establish the approximation theory for quasiperiodic functions with Diophantine frequencies across arbitrary dimensions. Moreover, it will introduce novel algorithms, namely the projection method and the finite point recovery method, designed to circumvent Diophantine errors. By leveraging the ergodic and arithmetic properties of irrational numbers, the mathematical underpinnings of these algorithms will be elucidated, extending the realm of high-precision numerical computations from the rational number field to the real number field. Time-permitting, applications in areas such as quasicrystals and their phase transitions, as well as grain boundaries, will be presented.

Acknowledgements: This work was partially supported by the National Key R&D Program of China (2023YFA1008802), the NSFC grants (12171412), and the High Performance Computing Platform of Xiangtan University.

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A novel variant of rhombic Penrose tiling

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It is well known that the Penrose tiling exists in three forms, namely, pentagonal tiling (P1), kite & darts tiling (P2), and rhombic tiling (P3) [1-3]. They are based on different prototiles and exhibit significantly different appearances. Still, they can be transformed into one another through local transformation rules; that is to say, the three tilings are mutually locally derivable [4]. We hereby report a new variant of rhombic tiling (hereafter referred to as P4) that is mutually locally derivable with the former three. Indeed, it has some excellent properties.

The P4 tiling (or simply P4) is composed of the two rhombic tiles as in P3. Although the arrangement of the rhombuses differs from P3, it is equally beautiful. The vertices of P4 are generated from five polygonal acceptance domains W_0, W_1, W_2, W_3 and W_4, which can be segmented into sections corresponding to seven kinds of vertex environments: D, Q, J, K, S, U, and W. Five of these environments (D, Q, J, K, S) are common with P3, while U and W replace T and V in P3. Specifically, W_0 (regular decagon) corresponds to the vertices, J, U, and W, incorporating acute vertices of the thin rhombus and generates the vertex set of P1. By adding the other four acceptance domains, W_1, W_2, W_3 and W_4, the vertex set of P4 is obtained.

The self-similarity of P4 under scaling by τ (the golden mean) is described using inflation rules for three thick and three thin rhombuses, distinguished by local configurations. This correlates with the fact that the Ammann bar grids (ABGs) as defined for P3, consisting of five sets of quasiperiodic line grids in five distinct orientations, intersect the rhombuses in P4 in six distinct manners. While the rhombuses in P3 are dual to the crossings between the ABGs [5], the rhombuses in P4 arise from the crossings in another grid pattern obtained by inverting the ABGs. The latter pattern consists of both straight lines and polylines. An assessment of the hyperuniformity order metric reveals that P4 compares better with P3 in its excellent hyperuniform properties.

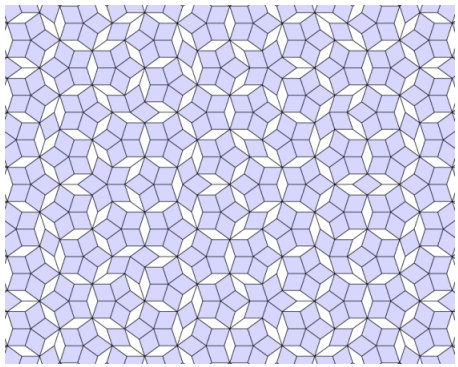

Fig.1: The P4 tiling, with thick (shaded) and thin (white) rhombuses.

Acknowledgements: Financial support from Japan Science and Technology Agency through CREST (Grant no. JPMJCR22O3) is gratefully acknowledged.

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Mathematical modelling of piezoelectric quasicrystals and quasicrystals

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Fundamental aspects of piezoelectric quasicrystals and quasicrystals are here addressed such as the constitutive modelling, the hyperspace notation, the three-dimensional as well as the two-dimensional Green tensors of arbitrary piezoelectric quasicrystals.
The basic framework of generalized piezoelectricity theory of quasicrystals will be presented by providing an improvement of the existing constitutive modelling [1]. It is shown that the tensor of phason piezoelectric moduli is fully asymmetric without any major or minor symmetry having important consequences in the constitutive relations as well as in its classification with respect to the crystal systems and Laue classes. The classification of the tensor of phason piezoelectric moduli with respect to the crystal systems and Laue classes is given for one-dimensional quasicrystals. The number of the independent components of the phason piezoelectric moduli is given for all 31point groups of one-dimensional quasicrystals. It is shown that 10 centrosymmetric crystallographic point groups have no piezoelectric effects and the remaining 21 non-centrosymmetric crystallographic point groups exhibit piezoelectric effects due to both phonon and phason fields.
In piezoelectricity of quasicrystals, where phonon, phason and electric fields exist, we introduce the corresponding multifields by developing the hyperspace notation for piezoelectric quasicrystals. Within the framework of linear piezoelectricity theory of quasicrystals, the three-dimensional and two-dimensional Green tensors for arbitrary piezoelectric quasicrystals are derived [2].
As subcase, the three-dimensional Green tensor for arbitrary quasicrystals is contained in the piezoelectric Green tensor of quasicrystals. For one-dimensional hexagonal quasicrystals of Laue class 10, which possess 10 independent material constants, a closed-form expression of the elastic 4 x 4 Green tensor is presented [3].
Moreover, the necessary and sufficient conditions for elastic stability and positive definiteness of the elastic energy density imposed on the elastic constants are given for one-dimensional hexagonal quasicrystals of Laue class 10 [4].

Acknowledgements: Markus Lazar and Eleni Agiasofitou gratefully acknowledge the grants from the Deutsche Forschungsgemeinschaft (Grant numbers LA1974/5-1, AG322/2-1).

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Lattice dynamics in quasicrystal i-AlPdMn and 1/1 approximant AgInYb

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Quasicrystals, characterized by aperiodic long-range order without translational symmetry, promise exotic physical properties beyond periodic crystals. While static quasicrystal structures have been well-studied using higher-dimensional spaces, their dynamic responses remain poorly understood. To explore lattice dynamics related to aperiodicity, we investigated low-energy phonons using neutron time-of-flight spectrometers DNA and AMATERAS at J-PARC. Our research focused on the quasicrystal i-AlPdMn and 1/1 approximant AgInYb.

Key findings in quasicrystal include hierarchical gap structures in acoustic modes scaled by the golden mean (Fig. 1), providing direct evidence of singular continuous states in aperiodic lattices. Additionally, phonon intensities in quasicrystals exhibited asymmetric behavior in energy and wave vectors relative to Bragg peaks, indicating characteristic nonreciprocal phonon propagation.

Comparative analysis with the periodic approximant crystal revealed critical differences. Intense dip structures at 5~8 meV intersecting the low-lying optical modes were observed, yet no hierarchical gap structures emerged below 5meV. Unlike the quasicrystal i-AlPdMn, the 1/1 approximant AgInYb crystal exhibited symmetric phonon intensities with nonreciprocal phonon propagation completely absent.

In this talk, we will discuss unique lattice dynamics of quasicrystals by comparing the phonon spectra in quasicrystals and periodic approximant crystals.

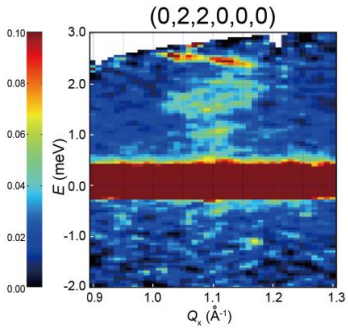

Fig.1: Contour maps of phonon scattering intensity of i-AlPdMn at *T*=300K [1].

Acknowledgements: This study was supported by JSPS KAKENHI Grant No.JP19H05819, No.JP19H05821 and JST-CREST Grants No.JPMJCR22O3.

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Phason dynamics for dodecagonal quasicrystals based on the elastodynamic model of wave-telegraph type

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In this work, phason dynamics is investigated by deriving the dispersion relations of two-dimensional dodecagonal quasicrystals of Laue class 18 based on the elastodynamic model of wave-telegraph type [1].
Two-dimensional dodecagonal quasicrystals provide a valuable platform to demonstrate the dynamic behaviour of the phason fields in quasicrystals, since the associated constitutive relations do not present a coupling between the phonon and phason fields [2]. According to the elastodynamic model of wave-telegraph type [3,4], which derivation is based on calculus of variations, phonon fields are represented by waves and phason fields are represented by waves damped in time and propagating with finite velocity. The damping character of the phason fields is achieved by considering phason frictional forces. Therefore, the equations of motion for the phonon fields are partial differential equations of wave type and for the phason fields are partial differential equations of telegraph type with the characteristic time of damping to be directly connected to the corresponding phason friction coefficient.
The dispersion relations for the phason displacement fields are analytically calculated for dodecagonal quasicrystals. It is found that there is a crucial threshold q_0, also called crossover, for the wavenumber, where the behaviour of the wave changes. The exact solutions are given covering the whole regime of possible wavenumbers of the phason fields. The phase and group velocities of the phason longitudinal and transverse waves are also calculated revealing that the phason waves are governed by an anomalous dispersion.

Acknowledgements: Eleni Agiasofitou and Markus Lazar gratefully acknowledge the grants from the Deutsche Forschungsgemeinschaft (Grant numbers AG322/2-1, LA1974/5-1).

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Soft and hard x-ray spectroscopies of magnetic Au-Al-Tb quasicrystal approximants

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The magnetism of rare-earth-based quasicrystals and their approximants is regarded as a new frontier in condensed matter physics, as novel magnetic properties and spin structures are expected to originate from quasiperiodic structures and icosahedral structures. The magnetic ground states of Au-Al-Tb approximants can be systematically tuned to exhibit antiferromagnetic, ferromagnetic, and spin glass states by the electron-per-atom (*e/a*) ratio [1,2]. Since the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the 4*f* electrons would be dominant in the Au-Al-Tb approximants, it is essential to clarify the valence electronic states, including 4*f* electrons, to understand the mechanism of this *e/a*-ratio dependence. In this study, we have investigated the valence electronic states of Au-Al-Tb approximants with different magnetic ground states in the paramagnetic phase.

The Tb 3*d*-edge resonance photoemission spectroscopy (RPES) has directly probed the Tb 4*f* states and revealed the dominant ionic-like localized Tb^{3+} states. On the other hand, the hybridization between the Tb 4*f* and 5*d* states just below the Fermi level (E_F) has been observed in the Tb 3*d*-edge RPES. The localized 4*f* electronic states have also been confirmed by the Tb 3*d* core-level hard x-ray photoemission spectroscopy (HAXPES). The *e/a*-dependent Au 5*d* electronic states have been observed by the valence-band HAXPES. Additionally, the *e/a*-dependent Au and Tb 5*d* electronic structures have been confirmed by the Au and Tb L_3-edge high-energy-resolution fluorescence detected x-ray absorption spectroscopy. The differences in valence electronic states around E_F would influence the differences in the magnetic ground states of the Au-Al-Tb approximants.

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Superconductivity in quasicrystal

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Quasicrystals, first discovered by Dan Shechtman [1], defy periodicity while exhibiting long-range order and high rotational symmetries. Their nontrivial structural characteristics have led to the discovery of unconventional electronic states, including anomalous transport [2]. Among the most recent breakthroughs is the experimental confirmation of bulk superconductivity in a Bergman-type Al-Mg-Zn quasicrystalline alloy in 2018 [3], evidenced by zero resistivity, Meissner effect, and specific heat jump at T_c=50mK. More recently, another superconductivity has been found in van der Waals quasicrystal $TaTe_{1.6}$ [4] (T_c=1K). These findings have opened the door to exploring superconductivity in aperiodic systems.

In this talk, I will present recent theoretical progress in understanding superconducting states in quasicrystals. Using real-space approaches such as the Bogoliubov–de Gennes method and real-space dynamical mean-field theory, we find that quasicrystals can host non-BCS-type superconductivity [5,6], including Cooper pairs with finite center-of-mass momentum. This leads to a finite paramagnetic current even at zero temperature [7,8].

These theoretical predictions are consistent with observed deviations from BCS expectations, such as reduced specific heat jumps in the superconducting state. I will also compare these superconductivity with small periodic approximants. This work based on a recent review [9], which provides a unified view of superconductivity in quasiperiodic systems across both experimental and theoretical domains.

Acknowledgements: N. T. is supported by JSPS KAKENHI Grant JP24K00585, 25H01400 and JST Grant Number JPMJPR23F6.

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Superconductivity of icosahedral approximants with Tsai-type clusters

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Strongly correlated electron systems have attracted much interest in studying unconventional superconductivity and non-Fermi-liquid states, related to magnetic quantum criticality. Quasicrystals possess long-range, quasi-periodic structures with diffraction symmetries forbidden to crystals. As a consequence of searching for superconductivity in quasicrystals, we have confirmed the emergence of bulk superconductivity of Al-Zn-Mg quasicrystal at a very low transition temperature of T_c = 0.05 K [1]. Furthermore, we have found two types of the Au-Ge-Yb approximants, which show superconductivity with transition temperatures T_c of 0.68 K and 0.36 K. The Tsai-type cluster center is occupied by Au and Ge ions in the former approximant, and by a Yb ion in the latter. For magnetism, the latter system shows a larger magnetization than the former [2]. Recently, noble superconductivity was discovered in 1/1 approximants with Tsai-type clusters, which exhibit unconventional superconductivity as observed in heavy fermion materials and strongly correlated electron systems. We present our low-temperature experiments on electrical resistivity, magnetization, ac magnetic susceptibility, and specific heat of the superconducting approximants. We also discuss possible unconventional superconductivity in these new systems.

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Electrical Resistivity of Quasicrystals Calculated from First Principles

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Electrical conductivity of quasicrystals has been calculated from first principles within electronic density functional theory. Realistic structure models containing up to 7,000 atoms were created utilizing empirical oscillating pair potentials for icosahedral AlCuFe and decagonal AlCoCu by Monte Carlo/molecular dynamics simulations as described in [1,2]. Intrinsic (T=0K) resistivity was evaluated using the Kubo-Greenwood formalism based on Green's functions calculated using the KKR multiple scattering method [3]. Icosahedral and decagonal models exhibited strong pseudogaps with the Fermi level lying within the gap. The icosahedral models show isotropic resistivity in the range of 800 microOhm-centimeters. The decagonal resistivity is anisotropic, with values of 700 in the quasiperiodic planes but less than 150 in the periodic direction. For the icosahedral quasicrystal, the resistivity as a function of Fermi energy is also calculated for the purpose of tunability.

Acknowledgements: This work was supported by NSF grant DMR-2103958 for development of resistivity calculation methods and DOE grant DE-SC0014506 for structure simulations. We used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

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Thermoelectric properties of icosahedral quasicrystals and 3/2 periodic approximants in the Al-Pd-TM-Fe (TM=Mo,W) systems

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Al-based icosahedral quasicrystals (i-QCs) are promising thermoelectric materials, capable of directly converting waste heat into electricity. The performance of thermoelectric materials is evaluated by the dimensionless figure of merit: $zT = \sigma S^2/\kappa$ (T: temperature, σ: electrical conductivity, S: the Seebeck coefficient, κ: thermal conductivity). Al-based i-QCs exhibit not only low κ, due to their complex crystal structures, but also high S, due to the presence of a deep pseudogap near the Fermi energy [1]. However, the criterion, $zT \geqq 1$, for practical applications has not yet been achieved in any Al-based i-QCs because of lower S than that of common commercial thermoelectric materials. Higher-order periodic approximants (PAs) provide valuable insights into the deepening pseudogap, potentially leading to an enhancement of S. In Al-Pd-(TM,Fe) (TM: Cr, Mo) systems, 3/2 PAs for Mackay-type i-QCs are stably formed [2,3]. Especially, with TM=Mo, two types of 3/2 PAs with similar compositions, designated as high temperature (HT) and low temperature (LT) phases with space groups $Pa\bar{3}$ and $P\bar{3}$, respectively, have been reported. For HT, a deeper pseudogap than that of i-Al-Pd-Mn was observed, suggesting that hybridization between Al-*sp* and TM-*d* orbitals contributes to the deepening pseudogap [5]. Recently, we revealed the stable formation of i-QC, HT, and LT in the TM=W system [4]. Herein, we focus on clarifying the effects of crystal structures and constituent elements on the depth of the pseudogap for HT and LT in the Al-Pd-(TM, Fe) (TM: Mo, W) systems.

Fig. 1 shows the temperature dependence of S for HT and LT with TM=Mo/W. HT exhibits higher S than LT regardless of TM, suggesting that the pseudogap of HT is deeper than that of LT. This can be explained by the difference in symmetry between HT ($Pa\bar{3}$) and LT ($P\bar{3}$). Meanwhile, HT (or LT) exhibits a similar maximum of S, with a slight shift depending on TM. In addition to these results, we will show the results of specific heat measurements, which allow for further insights into the effects of crystal structure and TM on the pseudogap.

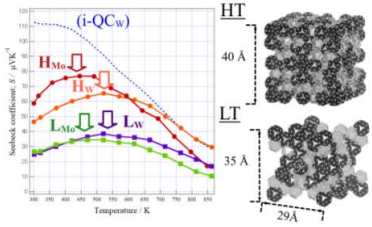

Fig.1: (left) the temperature dependence of the Seebeck coefficient S. The samples are expressed as H (or L) $_{\text{Mo or W}}$ (HT or LT with TM=Mo or W) (right) the crystal structure of HT and LT, visualized with VESTA [6].

Acknowledgements: This work is financially supported by Japan Science and Technology Agency through CREST (Grant no. JPMJCR2203)

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Long-range magnetic order in icosahedral quasicrystals

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Since the discovery of quasicrystals (QCs) in 1984 [1], one of the fundamental issues in the QC field has been to clarify whether long-range magnetic order (LRMO) exists in QCs. In this context, the discovery of rare-earth (R) containing QCs, such as Zn-Mg-R [2], Cd-Mg-R [3], and Cd-R [4] i QCs, opened up a new research field for investigating the magnetism of localized moments embedded in a quasiperiodic lattice. However, all R containing QCs commonly exhibited spin-glass behaviour, and no long-range magnetic order (LRMO) was observed. In contrast, Tsai-type 1/1 approximant crystals (ACs) were found to exhibit diverse magnetic orders, including ferromagnetic, antiferromagnetic, and spin-glass states [5].

Extensive research on Tsai-type ACs over the past decade has revealed that the magnetism of ACs can be well controlled by the electrons-per-atom (e/a) ratio [5,6]: Physical quantities such as the Weiss temperature (Θp) and the Curie temperature (Tc) are well described by the e/a ratio. Furthermore, studies on the magnetism of composition-tuneable Tsai-type 1/1 ACs have made it possible to significantly understand and predict the magnetism of Tsai-type QCs. The absence of LRMO in previously studied QCs is now explained by the fact that their e/a ratios are located in the strongly frustrating regime. Based on the magnetic phase diagram of ACs, new Au-Ga-R (R=Gd,Tb) QCs were synthesized in the ferromagnetic region by the melt-spinning method, and they were confirmed to exhibit ferromagnetic transitions as expected [7]. This marks the first observation of LRMO in QCs. Subsequently, a high-phase purity ferromagnetic Au-Ga-Dy QC with a wide single-phase region was also obtained [8]. More recently, antiferromagnetism was finally observed in Au-In-Eu QC [9], the reason of which is not fully understood yet. In this presentation, we will showcase our latest research findings on LRMO in both ACs and QCs and present the recent advancement.

Acknowledgements: This work was supported by JST CREST Grant Number JPMJCR22O3, JSPS KAKENHI Grant Numbers JP19H05817, JP19H05818, JP21H01044.

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Graphene-based moiré quasicrystals

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The ability to stack a few layers of graphene in a semi-controllable manner has opened new experimental avenues for exploring the physical properties of a novel class of quasicrystals—commonly referred to as *moiré quasicrystals* [1]. More broadly, this capability has sparked both theoretical and experimental investigations of two-dimensional quasicrystals constructed from periodically ordered atomic layers, with attention to both their geometric structure [2,3] and their emergent physical behavior. In this talk, I shall highlight several distinctive features of these systems that I believe will be of particular interest to the ICQ16 community.

Acknowledgements: I thank Aviram Uri and Sergio de la Barrera for numerous insightful discussions during our collaboration, and Meshy Ochana for her central contributions to our joint work. This research is supported by the Israel Science Foundation (ISF), grant no. 1259/22.

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The random tiling character of oxide quasicrystals

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Oxide quasicrystals (OQCs) are aperiodic 2D oxide films exhibiting dodecagonal symmetry, which are grown on hexagonal metal substrates. Their square-triangle-rhombus tilings are fromed by Ba, Sr, or Eu atoms hosted within a Ti-O network [1]. Recently, the tailor-made fabrication of OQCs has been demonstrated starting from hexagonal Ti_2O_3 honeycomb networks grown on Pt(111) and Pd(111) substrates. The deposition of Ba, Sr, and Eu up to a decoration of 73% of all honeycomb pores drives these periodic systems into perfectly-ordered dodecagonal tilings.
In this contribution, we present an internal space characterization of the three different oxide quasicrystal tilings in Ba-Ti-O/Pt(111), Sr-Ti-O/Pd(111) and Eu-Ti-O/Pd(111). By applying the novel geometric approach for a hyperspace analysis based on the evaluation of the real-space tilings derived from atomically-resolved STM images, we unambiguously prove the dodecagonal symmetry for all three systems [2]. By analysing the internal space point distributions we find some scattering of points out of the acceptance domain. However, the mean-squared expansions of the internal space clouds grows at very small slopes in dependence of the system size, compatible with a random tiling model. Furthermore, the absolute value of the Fourier transform of the largest OQC domain found for the Ba-Ti-O/Pt111 system exhibits a single oszillation surrounding the central peak, pointing to comparably high phason elastic constants in these random tiling quasicrystals [3].

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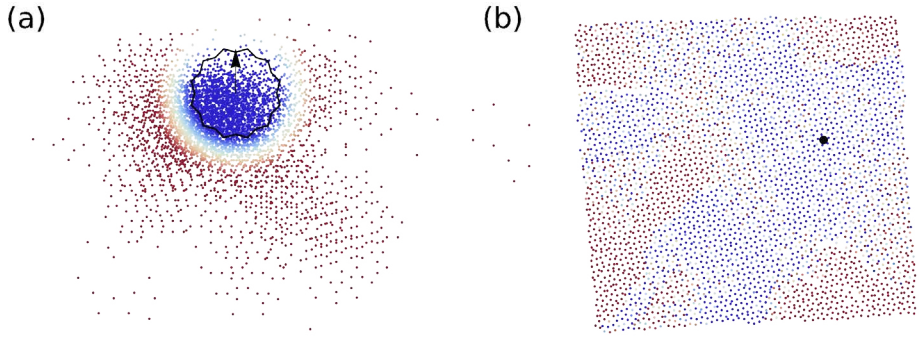

Fig.1: (a) Internal and (b) parallel space of the Sr-Ti-O OQC grown on Pd(111). Points are color-coded according to their distance from the center of the internal space. The black star in (a) labels the acceptance domain. The black dot in (b) marks the starting atom for the lift.

Analysis of Dislocations in Dodecagonal Oxide Quasicrystals

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We examine STM images of quasicrystals consisting of thin layers of Ba-Ti-O deposited on Pt(111) surfaces, forming two-dimensional dodecagonal quasicrystals [1]. We identify dislocations and calculate their Burgers vectors using an automated procedure, where we decompose the quasicrystal into individual density modes, or Fourier components, and determine the topological winding number associated with each mode [2,3].

We accompany this analysis of the data by performing numerical and analytical investigations of the effect of single dislocations on the profiles of Bragg peaks in the diffraction spectrum, utilizing both artificial and experimental datasets. Our findings reveal a qualitative way to distinguish between dislocations and other types of defects. Furthermore, we characterize the phason strain that is induced by dislocations in the quasicrystal, within the cut-and-project framework, by considering the degree of scatter, around the atomic surface, or acceptance domain, of the points projected onto perpendicular space.

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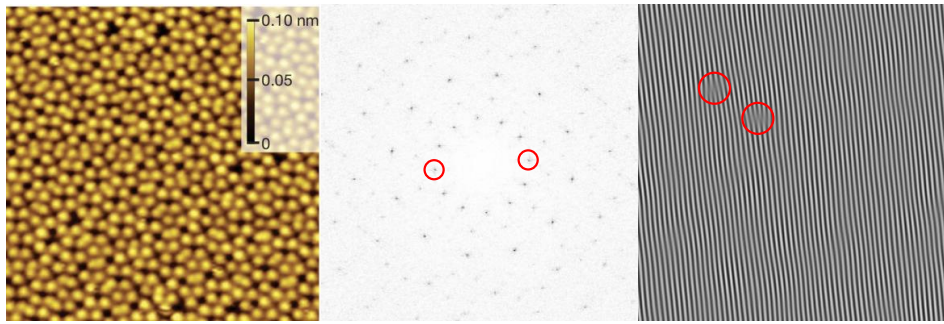

Fig.1: (a) Example of a segment from an STM image of a dodecagonal quasicrystal, of a Ba-Ti-O-derived thin film phase on Pt(111) [1], showing several dislocations. (b) Fourier transform of the atomic positions of an STM image from the same dataset, with the central peak blocked. A pair of Bragg peaks, associated with one of the basis vectors and its negative, is marked in red. (c) The corresponding section of the inverse Fourier transform of the filtered Bragg peaks marked in (b) with red circles marking the positions of two dislocations.

Intermetallic PdGa

From Chirality Transfer to the World Smallest Molecular Motor

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Intermetallic compounds (IMC) have gained significant interest in the last decade as highly active and at the same time very selective heterogeneous catalysts with potentially high stability. This interest originates from the large variety (thousands) of possible binary and ternary IMC and their widely ranging structural complexity (from a few to several hundreds of atoms in the unit cell). This allows tuning the valence electronic structure as well as the surface structure and therefore manipulating the so-called ligand effect (electronic structure effect) and the ensemble effect (atomic structure effect) on surfaces chemical reactions. Additionally, the space group of certain IMC reveal intrinsic chirality, which qualifies these materials for asymmetric heterogeneous catalysis/synthesis. Despite this great potential and the increasing amount of empirical investigations of catalytic properties of IMC, fundamental atomistic characterizations and understandings of the chemical processes on their surfaces is scarce.

In this talk, I would like to present atomic-scale reactant-catalyst interactions at low-Miller index surfaces of IMC PdGa with 1:1 stoichiometry. Owing to its non-centrosymmetry, PdGa exists in two enantiomorphs that are denoted PdGa:A and PdGa:B. Of particular interest are the two structurally different, threefold symmetric, chiral PdGa:A(-1-1-1)Pd_3 and PdGa:A(111)Pd_1 surfaces, which terminate by Pd trimers and isolated single Pd atoms, respectively. These surfaces have proven to be excellent candidates to separate the ensemble and ligand effect in heterogeneous catalysis and to exhibit highly enantiospecific interaction with achiral and prochiral molecules. Furthermore, PdGa has recently attracted considerable attention as topological material hosting exotic fermionic quasiparticles and as stator of the world smallest motor to date (cf. Fig.1).

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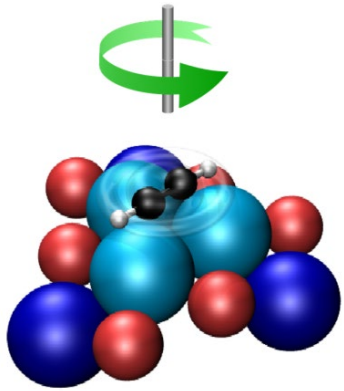

Figure 1: Sketch of the acetylene (C_2H_2) rotor on the atomic cluster structure of PdGa:A(-1-1-1)Pd_3 acting as chiral stator enabling unidirectional motion.

Ta–Te van der Waals layered quasicrystal: Synthesis of sub-millimeter scale single grains and synthesis of ternary systems

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Superconductivity in quasicrystals has been discovered in 2018 [1]. For Al–Zn–Mg icosahedral quasicrystal, convincing evidence indicated by zero resistivity, large diamagnetism, and specific heat jump, with a transition temperature 50 mK, has been presented. Recent theoretical studies on superconductivity in quasiperiodic systems predicted some unique characteristics. However, in order to experimentally explore the superconducting properties, superconducting quasicrystal with higher transition temperature is required. Recently, we found superconductivity in Ta–Te van der Waals (vdW) layered quasicrystal [2] at transition temperature $T_c \approx 1$ K [3]. Here, we report synthesis and superconducting properties of Ta–Te vdW layered quasicrystal.

The samples were prepared by reaction sintering. $TaTe_2$ and Ta powders were mixed at a mol ratio of 1:3 and compacted with a trace amount of iodine inside. Then, the mixture was sealed in an evacuated quartz tube, followed by heat treatment. The heat treatment was performed in two different conditions: The first is single-stage at 1,000°C, and the second is a two-stage process at 1,100°C and 1,450°C. The single-stage heat treatment resulted in grains with a diameter of tens to hundreds of μm on the quasiperiodic surface and a thickness of 1 μm in the periodic axis direction. On the other hand, the two-stage heat treatment resulted in grains with a diameter of several hundreds of μm on the quasiperiodic surface and a thickness of tens μm in the periodic axis direction. The possibility of measuring single crystal properties has greatly expanded due to the enlargement of grain size.

Recently, we also fabricate Ta–X–Te ternary systems, in which the third element X is added to Ta–Te binary system. So far, most ternary systems exhibit better crystallinity than Ta–Te binary system. The temperature dependence of the electrical resistance of single-phase quasicrystalline samples was measured and superconducting transitions were observed at ~1 K for all samples. It has been suggested that T_c is positively correlated with the density of states at the Fermi energy in the normal state.

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Relation between 1D quasicrystals and 2D Quantum Hall problems

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The extraordinarily precise quantization of the Hall conductivity which is well-known and used in metrology, is a consequence of topological properties of the band structure. Quasicrystals are topological systems. For quasicrystals, a well-known gap labeling theorem states that all spectral gaps are characterized by an integer, the gap label, having a topological origin [1]. One tangible result of the nontrivial topology are the edge states which appear on the edges of open chains. The same phenomena hold in higher dimensional systems, as shown in the figure below.
The relation of gap labels to electronic band structure in 1D quasicrystals has not thus far been clarified. Technically this is due to the fact that while gap labels can be deduced from the band Chern numbers, these latter cannot be computed directly for the 1D system. One possible solution is suggested by previous works by Zilberberg and collaborators who have noted the topological equivalence between the quasicrystal and the 2D Quantum Hall problem [2]. However an explicit connection between the two problems has not been provided thus far.
In this talk, I will show how to compute Chern numbers for bands in 1D periodic approximants of quasicrystals by taking a certain limit of a two-dimensional Quantum Hall problem. The model, which I call the Fibonacci-Harper model, provides the missing link between the two models.
The method will be explained for the Fibonacci chain, which is based on the golden mean irrational. There is an interesting topological (Lifshitz) transition along a line in the phase space of the model. This transition is marked by the change of Chern number, and the disappearance of edge states in open systems.
This approach also successfully yields the gap labels for another 1D quasicrystal, the silver mean chain. More excitingly, I will discuss how these models can be generalized to 2D and 3D quasicrystals, where higher order Chern numbers could be computed and related to experimentally measurable transport quantities.

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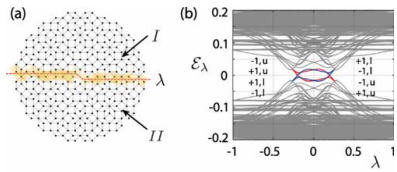

Fig.1: example of a surface state in a 2D quasicrystal (taken from Chen et al, PRR (2024)

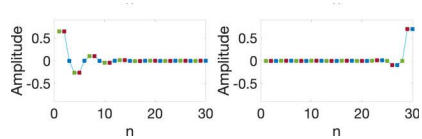

Fig.2: Edge states in a 1D chain for SSH3 model (taken from Anastasiadis et al, PRB (2022).

Magnetic phase diagrams of Tsai-type approximant crystals: From 1/1 to 5/3 approximant structures

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Tsai-type approximants share the same local atomic structure as quasicrystals, exhibiting properties of both quasicrystals and periodic crystals. Recent experiments have revealed various low-temperature magnetic phases, including spin glass, ferromagnetism, and antiferromagnetism [1]. The magnetism arises from localized moments on rare-earth ions located at icosahedral vertices in nested polyhedral clusters (Tsai-type clusters). These moments interact via the RKKY mechanism, with additional influence from crystal field anisotropy depending on the ion species. To assess the relative roles of RKKY interaction and anisotropy, we constructed a phenomenological effective spin model and found good agreement with experimental results, indicating that crystal field anisotropy dominates for some rare-earth elements [2].

In contrast, Gd-containing Tsai-type approximants are expected to exhibit negligible anisotropy due to the absence of orbital angular momentum. Nevertheless, various magnetic orders have been experimentally observed in such systems through compositional tuning [1]. To investigate this, we developed an effective model that considers only the RKKY interaction and assumes that compositional changes affect only the Fermi wavevector via variations in the electronic charge density. Using classical spin simulations based on the simulated annealing method, we successfully reproduced multiple magnetic phases consistent with experimental observations [3]. A comparison with the experimentally determined Weiss temperatures further confirmed the validity of our approach. We also performed a detailed analysis based on icosahedral clusters in the 1/1 approximant, showing that understanding the local magnetic configuration of clusters is crucial for elucidating the global magnetic order [4].

In this presentation, we extend our study to include 2/1, 3/2, and 5/3 approximants, which are structurally closer to quasicrystals. We present the resulting magnetic ground-state phase diagrams and discuss the similarities and differences with respect to the 1/1 approximant.

Acknowledgements: The authors acknowledge financial support from JSPS KAKENHI Grant Numbers JP19H05821, JP21H01044, and JP25H01399.

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Laser powder bed fusion of an approximant Au–Si–Gd phase reinforced Au matrix composite

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Using the laser powder bed fusion (LPBF) method, the composite materials with the structure in which Al-Fe-Cr quasicrystals are dispersed in an Al matrix exhibits excellent mechanical strength [1]. Furthermore, composites in which Au-(Si, Ge)-(Gd, La) quasicrystal/approximant crystal phases are dispersed in an Au matrix using spark plasma sintering (SPS) show higher hardness compared to the samples prepared by arc melting [2]. However, no reports of samples made using LPBF are available in which Au-based quasicrystal/approximant crystal phases are dispersed in an Au matrix. Therefore, the resulting microstructure and mechanical strength are of significant interest.

In this presentation, we will show samples with a structure in which Au-Si-Gd approximant crystals are dispersed in an Au matrix using the LPBF method. A 22-karat gold alloy powder with a composition of $Au_{83.18}Si_{8.97}Gd_{7.85}$ was prepared using gas atomization, and the average particle size was adjusted to 20 μm diameter through classification. The morphology of the cross-section of the particles was observed using field-emission scanning electron microscopy (FE-SEM), and the crystal structure was characterized using powder X-ray diffraction (XRD). We attempted to build cylindrical samples by additive manufacturing under various conditions of laser power, scanning speed, and hatch pitch. The SEM images show that the Au-Si-Gd phases were finely dispersed in the Au matrix, similar to the distribution observed in the powder. Additionally, XRD pattern peaks of the Au phase and the 1/1 approximant crystal phases were also confirmed (Figure 1a). Compared with the powder XRD peak pattern, clearer peaks were obtained, suggesting that the rapid cooling effect by local melting and solidification by the laser caused many approximant crystal phases to appear. This material was harder than the SPS materials reported by Shirota *et al.*, with an average hardness of 268 HV, indicating that dispersion strengthening likely occurred. Additive manufacturing, typified by the LPBF method, can produce shapes that are difficult to form using melt casting (Figure 1b), and it is hoped that applications that utilize these characteristics will be developed.

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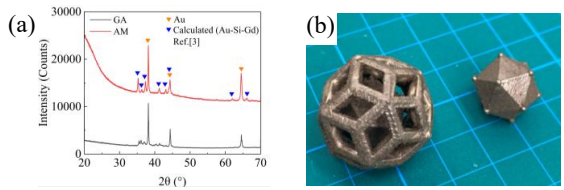

Fig.1: (a) XRD patterns of gas-atomized powders (GA) and additive manufactured materials (AM); (b) nested structure of an icosahedron and a rhombic triacontahedron (left), and the structure of an icosahedron only (right) prepared by LPBF.

Growth and properties of epitaxial CoCrFeNi high-entropy alloy thin films

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High-entropy alloys (HEAs) have attracted attention for a variety of applications. Among them are their application as structural materials, for radiation-exposed building parts in nuclear reactors as well as in the form of wear and corrosion protection layers. More recently they have also been proposed as effective electrocatalysts [1]. However, although the surface properties of HEAs play a central role for corrosion protection and catalysis, they are still largely unexplored. Fundamental studies of single-crystalline low-index surfaces of HEAs are extremely scarce [2]. This is - at least to a certain extend - caused by the unavailability of single-crystalline samples. One possibility to overcome this bottleneck is to use epitaxial films grown on single-crystalline substrates.

This presentation will summarize our recent work on the growth and subsequent characterization of epitaxial CoCrFeNi films [3]. The films were deposited by DC magnetron sputtering from spark-plasma sintered targets [4] onto single-crystalline oxide substrates. X-ray diffraction (XRD), scanning electron and transmission electron microscopy (SEM, TEM) and energy-dispersive X-ray spectroscopy (EDX) were employed to study the bulk properties of the deposited films. It was observed that face-centered cubic CoCrFeNi films grow epitaxially on MgO(100) and Al_2O_3(0001) substrates, exposing low-index (100) and (111) surfaces, respectively. A characterization of the surfaces was performed using X-ray photoelectron spectroscopy (XPS), angle-resolved photoelectron spectroscopy (ARPES), low-energy electron diffraction (LEED) and, more recently, scanning tunneling microscopy (STM). From these studies it can be concluded that epitaxially grown HEA films have the potential to fill the sample gap, allowing for fundamental studies of properties of and processes on well-defined HEA surfaces.

Acknowledgements: Funding by the European Social Fund (ESF) and the Free State of Saxony (via Sächsische Aufbaubank-Förderbank/SAB-100382175) as well as by the German Research Foundation DFG (project number 535729384) is gratefully acknowledged.

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Local Atomic Order in High-Entropy Alloys Studied by Atomic-Resolution Holography

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High-entropy alloys (HEAs) and quasicrystals both challenge the conventional paradigm of crystalline materials with simple, periodic unit cells. While quasicrystals exhibit aperiodic long-range order in three dimensions, HEAs typically adopt simple average structures (e.g., fcc or bcc lattices) but contain extreme chemical complexity due to multiple principal elements. However, they share several distinct physical properties, in particular regarding their (low) thermal conductivity, which is tied to their complex local atomic environments.

We explored the local atomic structure of a single-crystal Al-Co-Cr-Cu-Fe-Ni high-entropy alloy using atomic-resolution holography (ARH), complemented by X-ray and neutron diffuse scattering as well as X-ray absorption spectroscopy, and find substantial chemical short-range ordering, with only minimal lattice distortions.

By resolving the three-dimensional local atomic environment around selected atomic species, our findings provide new insights into the nature of chemical and structural disorder in HEAs and quasicrystals, aimed at establishing a new conceptual framework for interpreting structure–property relationships in both material classes.

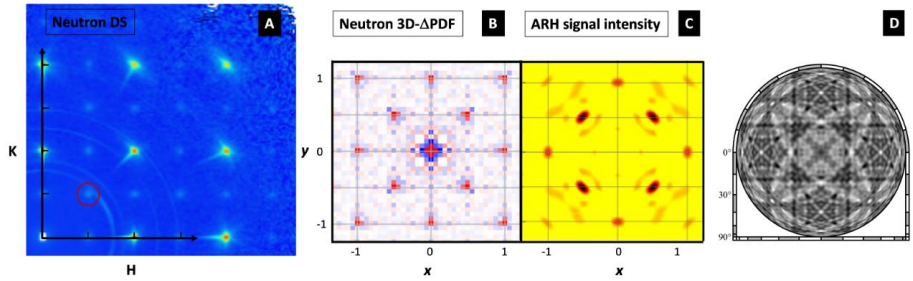

Fig. 1. a) HK0 map measured with neutron, the diffuse signal, circled in red, is on the site of the expected absences for an entropic FCC structure. The Fourier Transform (b) of the neutron 3D scattering, removing the signal from the Bragg peaks confirms the surplus of signal given by the anti-clustering behaviour of the elements. This can be compared to: c), the real-space reconstruction of an ARH simulation from a model (with an exemplary Ni hologram shown in d).

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Band structures in sonic quasicrystals

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For several decades, the physical properties of quasicrystals—such as electronic, vibrational, and photonic eigenvalue problems—have been a major research focus in the field of quasicrystals [1]. Here, we present the results of eigenvalue problems for "sonic quasicrystals" using the plane-wave expansion method and the finite element method [2]. Our sonic quasicrystals consist of dodecagonal quasiperiodic arrangements of 0.4 m diameter cylinders embedded in air. The bulk modulus of the cylinders is set to infinity.

Similar to photonic quasicrystals, sonic crystals exhibit band gaps that prevent certain frequencies of sound waves from propagating. Unlike 2D photonic crystals, which have TE and TM modes that complicate the formation of complete band gaps, sonic crystals have only one mode, making band gap formation easier. Since square and hexagonal lattices have been extensively studied in the field [2], we consider a series of square approximants of dodecagonal quasicrystals composed of squares and equilateral triangles, including the 33434 Archimedean tiling, with unit cells containing 4, 15, 56, and 209 cylinders.

We first find that these approximants exhibit multiple band gaps, all of which are similar to those of the 33434 Archimedean tiling. Fig.1(a) shows the band structure of the 33434 tiling in the frequency range of 0 Hz to 2100 Hz. The plane group of the 33434 tiling is *p*4*gm* with glide symmetry, where the eigenvalues along the X-M line are degenerate. Fig.1(b) displays the band structure of the 56-cylinder approximant that also has *p*4*gm* symmetry. Second, we observe that bandgap widths are strongly affected by even a small number of phason flips generated by "zipper moves" [3]. Finally, we find that these sonic quasicrystals exhibit several self-similar properties, akin to those of a 1D sonic quasicrystal.

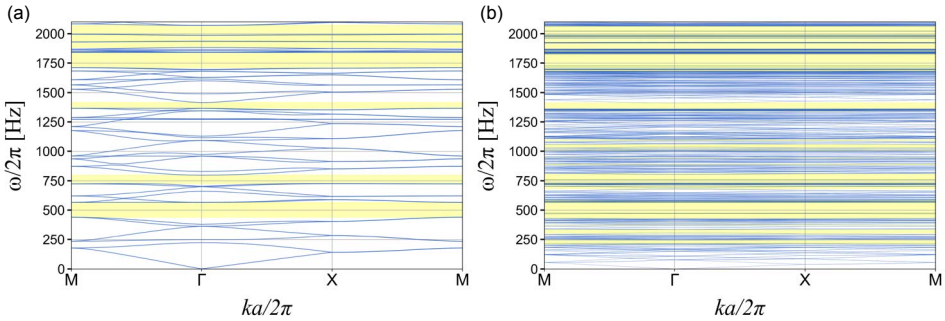

Fig.1: Sonic band structures: (a) 33434 Archimedean tiling and (b) 56-cylinder approximant of a dodecagonal quasicrystal.

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Cluster quasicrystals composed of ultrasoft particles vs. soft quasicrystals built of colloids with hard cores

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We study and compare two different approaches for the stabilization of soft quasicrystals.

First, we consider quasicrystals and other complex patterns that self-assemble in systems consisting of ultrasoft colloids that can completely overlap thus forming cluster crystal. Quasicrystals can be either stabilized by interactions with multiple length scales [1,2,3] or by preferred binding angles as in patchy colloids [4]. In a mean field approach the Lifshitz-Petrich-model [1,2] or a Phase Field Crystal Functional can be used to predict the structures.

Second, we study a system where the colloids cannot overlap. Either the colloids possess a soft core with at least a second length scale (e.g., as in [5]) or patchy colloids are considered [6]. A Density Functional Theory is implemented by using a variant of the Fundamental Measure approach [7] for the hard core.

While the ultrasoft particles assemble in cluster quasicrystals where the particles can completely overlap, the colloids with hard cores form structures that are rather dominated by the tiles that occur on a local level. To obtain specific quasicrystalline structure by designing the pair interaction, in case of ultrasoft particles the length scales in reciprocal space have to chosen appropriately (cf. [1,2,3]) while for colloids with hard cores the lengths in direct space have to be adjusted in order to obtain specific tiles (cf. [5]). Our results explain the differences and similarities between different types of quasicrystals and their design principles.

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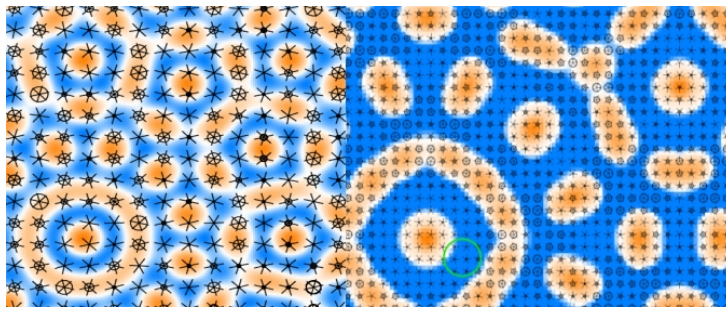

Figure: Dodecagonal patterns obtained by mean field calculations. Left: for ultrasoft particles with 6 patches [4]; Right: with hard cores and 5 patches per colloid.

Large-scale database analysis of anomalous thermal conductivity of quasicrystals and its application to thermal diodes

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One long-standing and crucial issue in the study of quasicrystals (QCs) has been to identify the physical properties characteristic of QCs. The large positive temperature coefficient of thermal conductivity $\lambda(T)$ at temperatures above room temperature, which has been observed in several QCs, is one such characteristic property. Takeuchi et al. conducted research on the development of high-performance thermal diodes that utilize this property [1, 2]. The thermal diode here has a structure in which materials with positive and negative temperature coefficients of $\lambda(T)$ are connected in series, and it has been shown that a thermal diode with a thermal rectification ratio (TRR: ratio of the magnitude of the forward and reverse heat flow) of up to 2.2 can be achieved by combining a QC with a positive coefficient and a material with an appropriate negative coefficient [1]. In this study, we analyzed a large physical property database "Starrydata [3]" to i) determine the degree of QC specificity with respect to the large positive temperature coefficient of $\lambda(T)$, and ii) search for the highest TRR thermal diode using QCs.

Starrydata contains approximately 23,500 $\lambda(T)$ curve data for various materials (metallic alloys, semiconductors, ceramics, etc.), and we analyzed 10,112 of these curves, which cover the temperature range of 300-600K.

Figure 1 shows the distribution of $R = \lambda(600\mathrm{K})/\lambda(300\mathrm{K})$ for all the 10,112 $\lambda(T)$ curves, where the arrows indicate the R values for QCs [4]. We can see that the QCs have particularly high R values among all materials. The largest R value for a QC is 3.2 for the Al-Cu-Fe system, which ranked nearly first. It was found that we can create a thermal diode with TRR=3.2 by combining this QC with an appropriately chosen crystalline phase [4]. This is the highest TRR among those reported to date for a solid-state composite thermal diode. Theoretical analyses are now underway to clarify the physical origin of the exceptionally large temperature coefficient of $\lambda(T)$ for QCs.

Acknowledgements: This study was supported by a JST CREST Grant (No. JPMJCR22O3), Japan, and KAKENHI Grant-in-Aid (No. JP19H05821) from JSPS.

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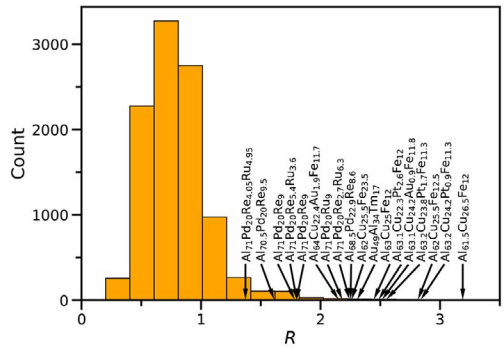

Fig.1: Distribution of the ratio of the thermal conductivities R=λ(600K)/λ(300K). Arrows indicate the R values for QCs.

Complex Dynamical Systems arising from Substitutions

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A symbolic random substitution assigns to each letter a finite set of possible images with a probability distribution producing complex dynamical systems with positive entropy [1, 2, 3], mixed spectral types [4], and nuanced mixing properties [5, 6]. In this study, we consider higher-dimensional random substitutions where each letter is mapped to a finite set of nonempty array of letters called rectangular words such that any letter can be iterated infinitely many times via the canonical concatenation to produce larger and larger rectangular words. We show that such systems are topologically transitive, have either empty or dense sets of periodic points, and have dense sets of linearly repetitive elements. For the case of primitive block random substitutions subshifts, we show that its inflation word entropy coincides with its topological entropy. We also show that the diffraction measure constant-shape random substitutions has a mixed spectral type consisting of a pure point part and an absolutely continuous part.

Acknowledgements: This research is funded under the National Research Council of the Philippines Grants-in-Aid and the University Research Council of Ateneo de Manila University.

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Diffraction of aperiodic monotile tilings

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The diffraction spectra of the recently discovered Hat and Spectre monotile tilings, which are known to be pure point, are derived and computed explicitly. This is done via model set representatives of self-similar members in the topological conjugacy classes of the Hat and the Spectre tilings, which are the CAP and the CASPr tiling, respectively. This is followed by suitable reprojections of the model sets to represent the original Hat and Spectre tilings, which consequently also allows to calculate their Fourier–Bohr coefficients explicitly. Since the windows of the underlying model sets have fractal boundaries, these coefficients need to be computed via an exact renormalisation cocycle in internal space. We provide a less technical introduction and present the main results such as the diffraction image of the Hat tiling around the origin (Fig. 1).

All results and their full derivation can be found in [1].

Acknowledgements: This work was supported by the German Research Council (Deutsche Forschungsgemeinschaft, DFG) under CRC 1283/2 (2021 - 317210226). AM also acknowledges support from EPSRC grant EP/Y023358/1.

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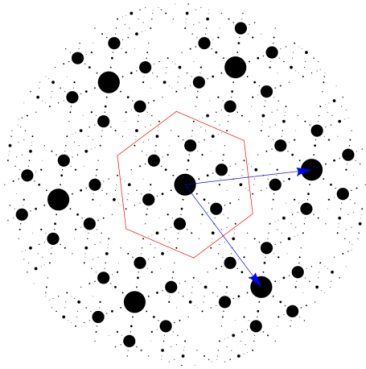

Non-ergodic phenomena in substituted intermetallics and alloys

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Randomness and frustrated interactions, the two requirements for spin-glass-like non-ergodic behavior, frequently appear in complex intermetallics. One common way in which this occurs is when pseudo-binary compounds are synthesized and the substitution either introduces randomness into the magnetic sublattice or into the magnetic interactions. The talk will start off by demonstrating non-ergodic behavior in two examples of complex metallic alloys, namely in the $Mn_xNi_2Zn_{11-x}$ pseudobinary γ- brass for $x = 0.3$ [1] and in the δ- $Co_{2.5}Zn_{17.5-x}Mn_x$ phase for $x = 0.4$ [2]. The systems have sufficiently high spin freezing temperatures of 16 K and 8 K, so that besides the zfc-fc magnetization splitting, the increased coercivity (in the spin-glass phase) and the shift of the AC susceptibility peak with frequency, also two more interesting experiments can be performed. The first revolves around thermoremanent magnetization – a phenomenon where a spin-glass-like system is cooled into the non-ergodic phase in an applied magnetic field and once the magnetic field is turned off, part of the magnetization decays towards zero extremely slowly, e.g. on the order of days, weeks or months. Secondly, in the memory-effect experiment one or several bits of information can be written into the spin-glass-like system without a magnetic field – by just temporarily stopping the cooling process at temperatures where we want to change the state of the system. On the warming cycle, magnetization is measured in a small applied magnetic field and small dips at the stopping temperatures show that the system has restored the state from the cooling run and has thus stored bits of information.

The second part of the talk will briefly discuss non-ergodic effects in high-entropy alloys, metallic systems composed of 5 or more principal elements. High-entropy alloys with their inherently high degree of randomness quite naturally fulfill the requirements for spin-glass-like behavior as soon as some AFM interactions appear besides FM interactions to also give frustration. We will start with two examples, where the high-entropy is single-phase, namely the hexagonal "ideal" Tb-Dy-Ho-Er-Tm HEA [3] and the fcc CoCrFeMnNi [4]. Finally, the two phase $Al_{28}Co_{20}Cr_{11}Fe_{15}Ni_{26}$ HEA [5] exhibits non-ergodic behavior only in the A2 nanoparticles.

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Complex magnetism of single-crystalline AlCoCrFeNi nanostructured high-entropy alloy

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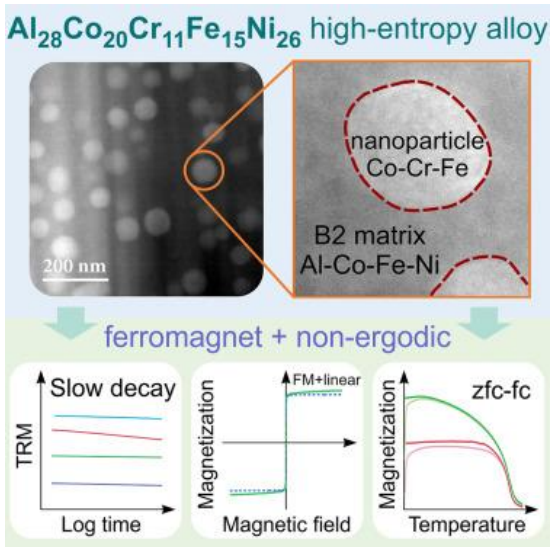
We have investigated magnetism of the $Al_{28}Co_{20}Cr_{11}Fe_{15}Ni_{26}$ single-crystalline high-entropy alloy. The material is nanostructured, composed of a B2 matrix with dispersed spherical-like A2 nanoparticles of average diameter 64 nm. The magnetism was studied from 2 to 400 K via direct-current magnetization, hysteresis curves, alternating-current magnetic susceptibility, and thermoremanent magnetization time decay, to determine the magnetic state that develops in this highly structurally and chemically inhomogeneous material. The results reveal that the Cr-free B2 matrix of composition $Al_{28}Co_{25}Fe_{15}Ni_{32}$ forms a disordered ferromagnetic (FM) state that undergoes an FM transition at 390 K. The Al- and Ni-free A2 nanoparticles of average composition $Co_{19}Cr_{56}Fe_{25}$ adopt a core-shell structure, where the shells of about 2 nm thickness are CoFe enriched. While the shells are FM, the nanoparticle cores are asperomagnetic, classifying into the broad class of spin glasses. Asperomagnetism develops below 15 K and exhibits broken-ergodicity phenomena, typical of magnetically frustrated systems [1].



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Phasons in the incommensurately modulated Rb_2ZnCl_4 phase

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Phason modes are one of the characteristic of aperiodic crystals. For all aperiodic crystals, the hydrodynamic theory predicts the occurrence of long wavelength phason modes , that are diffusive like excitations with a purely imaginary 'dispersion' relationship [1]. They have been observed in incommensurately displacive modulated structure, where propagating damped harmonic excitations are observed in a short wavelength regime, becoming overdamped excitations in the long-wavevlength limit. They have also been observed in quasicrystal and in this case diffusive excitations have been observed at all wavelength [2,3].This difference between the excitation spectrum of the two systems is intimately related to the microscopic realisation of phason modes: in one case phason modes results in small shift of atoms from their ideal position, whereas in the second case phason modes lead to atomic jumps.
We present the lattice dynamics study of the Rb_2ZnCl_4 phase which displays a crystal structure where the orientations of its $ZnCl_4$ tetrahedrons plays a crucial role. Whereas in the high temperature phase the tetrahedra occupy randomly two equivalent positions, from T_i=303 K they order incommensurately along the c* axis. The transition is related to the tetrahedron orientation and is of the order/disorder type. One thus expects diffusive phason modes at all wavelength, as predicted by the theory [2,3]. At T_C=195K the modulation gets locked-in with a 1/3 ratio of the periodicity at high temperature, resulting in a periodic approximant, where phason modes should not be present anymore.
We have investigated the dynamics of this phase, as a function of temperature between 140 and 350 K, using inelastic and quasielastic neutron scattering measurement on a large single crystal,
In the incommensurate phase, a strong quasielastic signal is observed only around satellites reflection. It presents a q dependence with a width that increases as q increase in agreement with the hydrodynamic theory of phason modes. We also observe broad and dispersive phonon like excitations in a restricted momentum-energy space. Only regular acoustic modes are observed around the main reflexions. In the lock-in phase at 150 K the quasielastic signal around the satellites reflexion has vanished and only acoustic phonon modes are observed. This demonstrates that phason modes are indeed a characteristic excitation of the incommensurately modulated Rb_2ZnCl_4 phase.

Acknowledgements: This work is part of the ANR-DFG Aperiodic project.
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“Self-compression” and thermal lock-in phase transition in an aperiodic composite crystal

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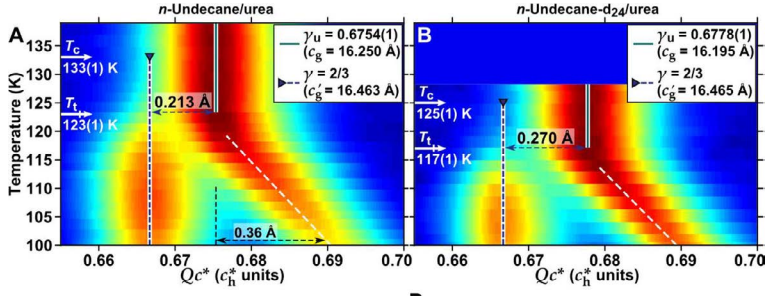
Since 1992, the new definition of the crystal includes materials which present long range order without translational symmetry. They are described within higher dimensional spaces, where they recover this lost translational periodicity. The physical space is then a 3-dimensional cut of this higher dimensional space. There is an infinite degeneracy of the ground state energy (“Mexican hat” potential), at the origin of very new fundamental physical properties (sliding modes). Examples by construction are quasicrystals [1] and aperiodic composite crystals [2,3].

We present thermal “selective compressibility” in the guest/host *n*-undecane/urea crystal. Opposite to pressure induced selective compressibility [4], it yields *an expansion* of the guest periodicity with *a simultaneous thermal-induced lock-in* of parts of the crystal at low temperature. These long-range ordered commensurate domains generate enough stress to “*self-compress*” other parts of the crystals along the aperiodic direction, defining a new type of solid-state phase transitions [5].



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[5] To be published.

POSTERS

POSTER EXHIBITION

P1	**AI-based search for semiconducting quasicrystals** **Kaoru Kimura**[1], Minoru Kusaba[1], Yutaka Iwasaki[2], Erina Fujita[1,2], Takanobu Hiroto[2], Asuka Ishikawa[3], Chang Liu[1], Yukari Katsura[2], Ryuji Tamura[3], Ryo Yoshida[1,2] *1-The Institute of Statistical Mathematics (ISM), Midori-cho, Tachikawa, Tokyo, Japan* *2-National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan* *3-Department of Materials Science and Technology, Tokyo University of Science, Katsushika,Tokyo, Japan*
P2	**Stability of diverse dodecagonal quasicrystals in T-shaped liquid crystalline molecules** **Xin Wang**[1], An-Chang Shi[2], Pingwen Zhang[3,4], Kai Jiang[1] *1-Hunan Key Laboratory for Computation and Simulation in Science and Engineering, Key Laboratory of Intelligent Computing and Information Processing of Ministry of Education, School of Mathematics and Computational Science, Xiangtan University, Xiangtan, Hunan, China,* *2-Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada* *3-School of Mathematics and Statistics, Wuhan University, Wuhan, China* *4-School of Mathematical Sciences, Peking University, Beijing, China*
P3	**Synthesis of Ga-Pd-RE (RE = Sm, Gd-Tm) i-QC by melt spinning** **Rei Naito**[1], T. D.Yamamoto[1], F. Labib[2], A. Ishikawa[2], R. Tamura[1] *1-Tokyo Univ. of Science, 6-3-1 Nijuku, Katsushika City, Tokyo, Japan* *2-Res. Ins. of Sci. and Tech., Tokyo Univ. of Sci. 6-3-1 Nijuku, Katsushika City, Tokyo, Japan*
P4	**HYPOD-X: Comprehensive experimental datasets of quasicrystals and their approximants** **Erina Fujita**[1,2], Chang Liu[1], Asuka Ishikawa[3], Tomoya Mato[2], Koichi Kitahara[4], Ryuji Tamura[3], Kaoru Kimura[1,2], Ryo Yoshida[1,2,5], Yukari Katsura[2,6,7] *1-The Institute of Statistical Mathematics (ISM), Research Organization of Information and Systems, Tachikawa, Tokyo 190-8562, Japan* *2-National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, Japan* *3-Department of Materials Science and Technology, Tokyo University of Science, Katsushikaku, Tokyo, Japan* *4-Department of Materials Science and Engineering, National Defense Academy, Yokosuka, Kanagawa, Japan* *5-Graduate University for Advanced Studies, SOKENDAI, Tachikawa, Tokyo, Japan* *6-Graduate School of Science and Technology, Tsukuba University, Tennodai, Tsukuba, Ibaraki, Japan.* *7-RIKEN Center for Advanced Intelligence Project, RIKEN, Chuo-ku, Tokyo, Japan*
P5	**Chiral spiral cyclic twins** **W. Hornfeck** *FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Prague, Czech Republic*

P6	**Computing the symmetries of kk-free lattice systems from imaginary biquadratic number fields** **M.L. Loyola**, K.A.C. de los Santos, E.D. Miro *Department of Mathematics, Ateneo de Manila University, Quezon City, Philippines*
P7	**Numerical Methods for Quasiperiodic Systems and their Applications in Schrödinger Operators** **Q. Zhou**, K. Jiang *Mathematics and Computational Science, Xiangtan University, Xiangtan, Hunan, China*
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P9	**Symmetries of a Symbolic Dynamical System Arising from a Biquadratic Number Field** **K. de los Santos**, M. Loyola, E. Miro *Department of Mathematics, Ateneo de Manila University, Quezon City, Philippines*
P10	**Tiles from projections of the root and weight lattices of A_n** **N. Ozdes Koca**[1], M. Koca[2], Rehab Ahmed Nasser Al Reasi[1] *1-Department of Physics, Sultan Qaboos University, Al Khoud, Muscat, Oman* *2- Professor Emeritus, Department of Physics, Sultan Qaboos University, Al Khoud 123, Muscat, Oman*
P11	**Theoretical studies of an artificial spin ice on the Ammann-Beenker tiling** **E. Weightman**, L. O'Brien, S. Coates *Department of Physics, University of Liverpool, Liverpool, UK*
P12	**Non-ergodic states in icosahedral quasicrystals Zn-Mg-*RE*(*RE*= Tm, Er, Ho)** **S. Vrtnik**[1,2], P. Koželj[1,2], A. Jelen[1], J. Luzar[1], J. Petrović[1], I. Buganski[3], R. Strzałka[3], J. Dolinšek[1,2] *1-J. Stefan Institute, Jamova 39, Ljubljana, Slovenia* *2-University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia* *3-AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, Krakow, Poland*
P13	**Single electrons on the Fibonacci quasicrystal: an interpolation between models** **A.M. Rucklidge**[2], R. Lifshitz[1], J. Niesen[2] *1-School of Physics & Astronomy, Tel Aviv University, Tel Aviv, Israel* *2-School of Mathematics, University of Leeds, Leeds, United Kingdom*

P14	**Synthesis and thermoelectric properties evaluation of Al-Ge-Ru 1/0 approximant crystals** **Y. Niwa**[1], Y. Iwasaki[2], K. Kitahara[3], T. D. Yamamoto[1], A. Ishikawa[4], K. Kimura[5], R. Tamura[1] *1-Dept. of Mater. Sci. & Tech. Tokyo Univ. of Sci., Tokyo, Japan* *2-NIMS, Tsukuba, Japan* *3-NDA, Yokosuka, Japan* *4 -Res. Inst. for Sci. & Tech. Tokyo Univ. of Sci., Tokyo, Japan* *5-ISM, Tachikawa, Japan*
P15	**Physical properties of supersilent high-entropy alloys** **J. Luzar**[1], S. Vrtnik[1,2], P. Koželj[1,2], J. Petrović[1], A. Jelen[1], P. Priputen[3], J. Dolinšek[1,2] *1-Jožef Stefan Institute, Ljubljana, Slovenia* *2-University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia* *3-Slovak University of Technology, Faculty of Materials Science and Technology, Bratislava, Slovak Republic*
P16	**A Julia Software Suite for Crystallography in Arbitrary Dimensions** **P. Kalugin** *Laboratoire de Physique des Solildes - UMR 8502, CNRS, Université Paris-Saclay, Orsay, France*
P17	**Synthesis and structure analysis of ZnMgEr P-type quasicrystal** **R. Strzałka**[1], I Bugański[1], J. Wolny[1], J. Kusz[2], N. Fujita[3] *1-AGH University of Krakow, Faculty of Physics and Applied Computer Science, Krakow, Poland* *2-University of Silesia, Faculty of Science and Technology, Katowice, Poland* *3-Tohoku University, Institute of Multidisciplinary Research for Advanced Materials, Sendai, Japan*
P18	**Vertex environments in the extended canonical cell tiling** **N. Fujjita** *Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan*
P19	**Pd-doped $Al_{13}Fe_4$ as an efficient catalyst for the semihydrogenation reaction of acetylene** **N. Fujita**[1], M. Hanaoka[1], E. Gaudry[2], K. Nozawa[3], S. Kameoka[1] *1-Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan* *2- Institut Jean Lamour, Université de Lorraine, UMR7198-CNRS, Campus ARTEM, Nancy, France* *3-Department of Physics and Astronomy, Kagoshima University, Korimoto, Kagoshima, Japan*
P20	**Structural investigation of the Ho-Au-Si (100) approximant surface** **W. Bajoun Mbajoun**[1], G. H. Gebresenbut[2], E. Gaudry[1], C. Pay Gómez[2], J. Ghanbaja[1], V. Fournée[1], J. Ledieu[1] *1-Institut Jean Lamour, Université de Lorraine, UMR7198-CNRS, Campus ARTEM, Nancy, France* *2-Uppsala University, Ångström Laboratory, Uppsala, Sweden*
P21	**Surface structure of Nd-Fe-B permanent magnets.** **A. Suresh**, W. Bajoun Mbajoun, G. Lengaigne, J. Ledieu, V. Fournée *Institut Jean Lamour, Université de Lorraine, UMR7198-CNRS, Campus ARTEM, Nancy, France*

AI-based search for semiconducting quasicrystals

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The presence or absence of semiconducting quasicrystals is a fundamental question in solid-state physics, and if they exist, they have the potential to become high-performance thermoelectric materials [1]. We have been searching for 35 years and have not yet to find it. Therefore, we are conducting a search using AI, which has advanced rapidly in recent years. First, we developed an AI (T_{SAI}) that predicts the composition of quasicrystals [2] and discovered three new quasicrystals [3]. After that, the composition of the semiconducting quasicrystal was predicted by learning more composition of quasicrystals in HYPOD-X (comprehensive experimental datasets of quasicrystals and their approximants, Figshare, https://doi.org/10.6084/m9.figshare.25650705.v3 (2024)) [4] and the temperature dependence of electrical conductivity and thermal conductivity in Starrydata (a database compiled from graphs in past papers: https://www.starrydata2.org/) [5]. Semiconducting quasicrystals are difficult to predict because they are in the extrapolation region of prediction. However, we have found a semiconducting approximants (crystals that have the same structural units as quasicrystals) [6,7], and the absolute value and temperature dependence of electrical conductivity of past quasicrystals and approximants are distributed continuously from typical metals to typical semiconductors, and we believe that it is not impossible to predict semiconducting quasicrystals by learning this trend. In the presentation, we will introduce the current state of experiments in the search for semiconducting quasicrystals.

Acknowledgements: This work was supported by the Grants-in-Aid for Scientific Research on Innovative Areas (19H05817, 19H05818, 19H05820), JSPS KAKENHI grant number JP23K26367 and the JST-CREST project (JPMJCR22O3).

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Stability of diverse dodecagonal quasicrystals in T-shaped liquid crystalline molecules

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Quasicrystals are intriguing ordered structures characterized by the quasi-periodic translational and non-crystallographic rotational symmetry. The tiling of different geometric units such as triangles and squares in two-dimensional space can result in a great variety of quasicrystals that could be realized by the self-assembly of liquid crystalline molecules. In this study, we introduce three self-similar dodecagonal tilings, including a novel Diamond-Square-Triangle pattern, composed of triangular and quadrangular tiles and examine their thermodynamic stability by using the self-consistent field theory applied to T-shaped liquid crystalline molecules. Specifically, we detail the inflation rules for the construction of these dodecagonal tilings and analyze their self-similarity, and show that these tilings can be viewed as projections of higher-dimensional periodic lattice points with projection windows. Using these dodecagonal tilings as initial configurations of the SCFT results in solutions corresponding to quasicrystals that could form from the T-shaped liquid crystalline molecules. The relative stability of these aperiodic phases is analyzed to obtain design rules that could stabilize quasicrystals. Meanwhile, we provide a criterion for distinguishing three dodecagonal quasicrystals and their approximants by analyzing their diffraction peaks. These findings shed new lighten on the discovery of new quasicrystals in soft materials.

Acknowledgements: This work is partially supported by the National Key R&D Program of China (2023YFA1008802), the National Natural Science Foundation of China (12171412), the Science and Technology Innovation Program of Hunan Province (2024RC1052), the Innovative Research Group Project of Natural Science Foundation of Hunan Province of China (2024JJ1008), and the Natural Sciences and Engineering Research Council of Canada.We are also grateful to the High Performance Computing Platform of Xiangtan University for partial support of this work.

Synthesis of Ga-Pd-RE (RE = Sm, Gd-Tm) i-QC by melt spinning

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Quasicrystals (QCs) have attracted a great deal of attention as a new platform for exploring novel magnetism due to the recent discoveries of quantum critical phenomena [1] and long-range magnetic orders [2-4]. These achievements have been made in Tsai-type icosahedral QCs (*i*-QCs), especially in Au-based alloys, motivating further explorations of new *i*-QCs in Tsai-type compounds. In this regard, the Ga–Pd–RE system (RE = rare-earth) is one of the interesting candidates because it is the only non-Au-based Tsai-type compounds in which antiferromagnetic 2/1 approximant crystal has been reported [5]. However, to the best of our knowledge, there is only the report in this system on the synthesis of Ga–Pd–Sc *i*-QC [6]. Hence, this study is aimed at thoroughly exploring new Tsai-type *i*-QCs in the Ga-Pd-RE system.

For synthesis of *i*-QC samples, the mother alloys of Ga-Pd-RE (RE = Nd, Sm, Gd-Tm) were prepared using a conventional arc-melting method under Ar atmosphere. The resulting alloys were then rapidly quenched by using a single-roller melt-spinning technique, where roll speeds were at 3500 and 4000 rpm. Powder X-ray diffraction (PXRD) measurements were performed using a Rigaku SmartLab SE for the phase identification of the melt-spun samples.

Fig. 1 shows the PXRD patten of the melt-spun samples in the Ga-Pd-RE (RE = Tb, Ho, and Tm) alloys. All the peaks can be indexed as *i*-QC peaks, suggesting the formation of a single-phase *i*-QC. Similar PXRD patterns are also observed for other Ga-Pd-RE alloys, except for RE = Nd, indicating the successful syntheses of Ga-Pd-RE (RE = Sm, Gd, Tb, Dy, Ho, Er, Tm) *i*-QCs. Furthermore, it is found that the width of the XRD peaks decreases with decreasing the atomic radius of RE element (r_{RE}), indicating that the crystallinity of these *i*-QCs is improved as $r_{\mathrm{RE}}/r_{\mathrm{others}}$ decreases, where r_{others} is the weighted average atomic radius of the other elements. This result suggests that the Ga-Pd-RE *i*-QCs would be thermodynamically stabilized by elemental substitutions to reduce the $r_{\mathrm{RE}}/r_{\mathrm{others}}$.

Acknowledgements: This work was supported by JSPS KAKENHI Grant Numbers JP19H05817, JP19H05818, and JP21H01044.

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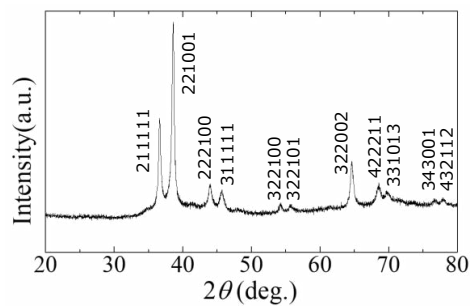

Fig. 1: Powder X-ray diffraction pattern (PXRD) of the Ga–Pd–Tb alloy

HYPOD-X: Comprehensive experimental datasets of quasicrystals and their approximants

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In this study, we have developed a comprehensive dataset, HYPOD-X, focusing on quasicrystals and approximants. This open dataset aims to address the lack of data in the field of quasicrystals and support data-driven materials discovery and machine learning. The dataset is constructed through an extensive literature survey and data extraction. The **Composition dataset** includes 915 compositions of quasicrystals, 525 compositions of approximant crystals, and 8 compositions categorized as either quasicrystals or approximant crystals, with each compsosition accompanied by structural types, sample preparation methods, and relevant references. Additionally, the **Phase region dataset** has been developed by digitizing data extracted from 43 ternary alloy phase diagrams, providing detailed compositional information. Furthermore, we have compiled temperature-dependent property data for 925 quasicrystals and approximants, covering electrical resistivity, Seebeck coefficient, thermal conductivity, and magnetic susceptibility, and systematically organized them into the **Properties dataset**. The data collection for the Properties dataset was facilitated using Starrydata2 web system[1], enabling efficient extraction and organization of literature data. These datasets comprehensively provide composition, structure, and property information for quasicrystals and approximants. HYPOD-X integrates over 40 years of data from quasicrystal research and is expected to serve as a foundation for data-driven-based new material exploration and property analysis. The constructed dataset is publicly available [2], allowing researchers easy access and utilization. This initiative is anticipated to deepen the understanding of quasicrystals and related materials, accelerating further material design and the discovery of novel functionalities.

Acknowledgements: This work was supported by the Grants-in-Aid for Scientific Research on Innovative Areas (19H05817, 19H05818, 19H05820), and the JST-CREST project (JPMJCR22O3).

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Chiral spiral cyclic twins

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The binary intermetallic glass-former NiZr exhibits tenfold cyclic Z module twinning, which arises from the nucleation of a decagonal quasicrystalline seed, and its subsequent growth into a twinned dendritic microstructure, upon the alloy's solidification from the deeply undercooled melt, as processed by the containerless electrostatic levitation method.[1,2]

An atomistic model can be derived based on the CrB type crystal structure of NiZr, with local atomic environments observed at the twin domain boundaries being identical to the bulk phase.[3]

The model can be studied for its own purpose, being generalized to a four-parameter family of (chiral) cyclic twins, based on a n-fold ($n > 4$) composition of discrete circle involute spirals, originating from highly regular integer sequences as their basic structure encoding principle. Special choices of the integer parameters yield all three regular periodic tilings of the plane, as well as aperiodic tilings based on rhombuses, related to the quasiperiodic tilings of Ammann-Beenker ($n = 8$), Penrose ($n = 10$), and Stampfli ($n = 12$).[4,5]

Acknowledgements: W.H. is grateful for the continuous endorsement by Michal Dušek.

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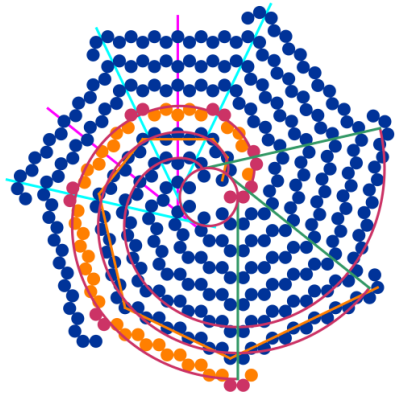

Computing the symmetries of k-free lattice systems from imaginary biquadratic number fields

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We consider a two-dimensional binary shift space X derived as the closure under the action σ induced by the lattice translations or shift maps of k-free points in the imaginary biquadratic number field $\mathbb{Q}(\sqrt{m}, i)$, where $m > 2$ is some positive integer, of class number 1 [1].

We are interested in the set of all homeomorphisms on X that commute with every shift map and those that normalize the group of all shift maps, called the automorphism group and the extended symmetry group, respectively, of the k-free lattice system (X, σ). It has been shown that the automorphism group of (X, σ) is trivial being composed only of the shift maps [2]. Following the methods in [2, 3, 4], we employ a direct computational approach to determine the extended symmetry group of (X, σ). Specifically, we show that it is the semidirect product of the automorphism group with the stabilizer of the k-free set of the number field.

Acknowledgements: This research is funded under the National Research Council of the Philippines Blue Skies Program and the Ateneo de Manila University Research Council.

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Numerical Methods for Quasiperiodic Systems and their Applications in Schrödinger Operators

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Quasiperiodic systems exhibit unique structures between periodicity and disorder, presenting fundamental challenges for conventional numerical approaches due to their full-space ordering dominated by irrational numbers, along with the absence of translational invariance and decay properties. We develop two innovative numerical methods for quasiperiodic systems and apply to quasiperiodic Schrödinger eigenproblems (QSEs): (1) We propose a new algorithm, the irrational-window-filter projection method (IWFPM) [1], for quasiperiodic systems with concentrated spectral point distribution. Based on the projection method (PM), IWFPM filters out dominant spectral points by defining an irrational window and uses a corresponding index-shift transform to make the FFT available. We apply IWFPM to 1D, 2D, and 3D QSEs to demonstrate its accuracy and efficiency. IWFPM exhibits a significant computational advantage over PM for both extended and localized quantum states. More importantly, by using IWFPM, the existence of Anderson localization in 2D and 3D QSEs is numerically verified. (2) We propose a new algorithm, finite points recovery (FPR) method, which is available for both continuous and low-regularity cases. The FPR method first establishes a homomorphism between the lower-dimensional definition domain of quasiperiodic function and the higher-dimensional torus, then recovers the global quasiperiodic system by employing interpolation technique with finite points in the definition domain without dimensional lifting. Numerical experiments demonstrate the effectiveness and superiority of FPR approach in recovering both continuous quasiperiodic functions and piecewise constant Fibonacci quasicrystals.

Acknowledgements: This work was partially supported by the National Key R&D Program of China (2023YFA1008802), the NSFC grants (12171412), and the High Performance Computing Platform of Xiangtan University.

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On the Spectrum of the Random Fibonacci Direct Product Variation

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We can describe the direct product of two Fibonacci tilings with four prototiles labelled by the numbers $0, 1, 2, 3$ with inflation rule ϑ given in Figure 1(a), where (intervals) a and b are of length $\tau = (1 + \sqrt{5})/2$, respectively. Note that the images of three prototiles under ϑadmit several decompositions – protile 2 and 3 have two decompositions while prototile 3 has 12 decompositions. This leads to 48 different inflation rules called the Fibonacci direct product variation (DPV). Figure 1(b) shows one Fibonacci DPV inflation rule.

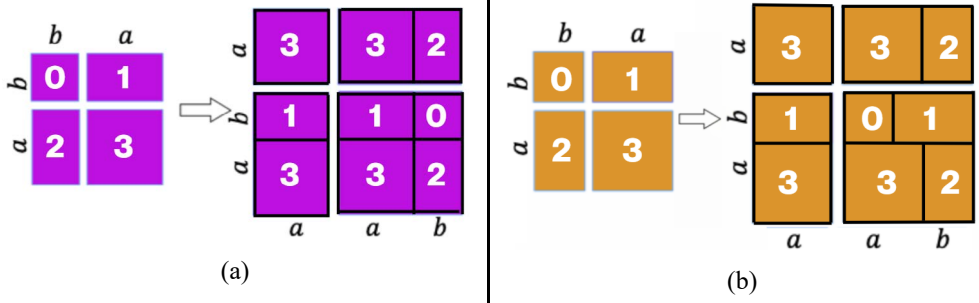

Figure 1. (a) The direct product of two Fibonacci inflation rule. (b) One of the 48 Fibonacci DPV inflation rules.

In this work, we consider the random version of the Fibonacci DPV where at least one prototile is mapped to at least two decompositions of its image. We show that this random substitution is of mixed spectral type consisting of a pure point part, corresponding to the discrete part, and an absolutely continuous part, corresponding to the fluctuations. Moreover, using Mathematica 14, we provide some visualizations for these distinct parts and look at the interaction between them.

Acknowledgements: This research is funded under the National Research Council of the Philippines Grants-in-Aid and the University Research Council of Ateneo de Manila University.

Symmetries of a Symbolic Dynamical System Arising from a Biquadratic Number Field

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We study the symmetries of a symbolic dynamical system (X, σ) of number-theoretic origin. Specifically, we consider the shift space X derived as the closure of k-free points in the ring of integers of the biquadratic number field $Q(\sqrt{2}, i)$ under the shift map σ. We are interested in the set of all homeomorphisms on X that commute with every element of the shift group ⟨σ⟩ and those that commute with the whole of the shift group ⟨σ⟩ called the symmetry group $\mathrm{Aut}(X, \sigma)$ and the extended symmetry group $\mathrm{Sym}(X, \sigma)$, respectively. It has been shown that the symmetry group $\mathrm{Aut}(X, \sigma)$ is minimal being composed only of the shift maps [1]. Using the underlying divisibility properties of the ring as in [1, 2, 3], we show that the extended symmetry group $\mathrm{Sym}(X, \sigma)$ is a semidirect product of the symmetry group with the stabilizer of the k-free set of the number field.

Acknowledgements: This study was funded by the Department of Science and Technology - Science Education Institute through the Accelerated Science and Technology Human Resource Development Program and the National Research Council of the Philippines Blue Skies Program.

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Tiles from projections of the root and weight lattices of A_n

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The 2D faces of the root lattice A_n and the weight lattice A_n^* $(n = 1,2, \dots)$ are projected onto the Coxeter plane displaying $(n+1)$ - fold symmetric tilings. The orbits of the fundamental weight vectors $\omega_1, \omega_2, \dots, \omega_n$ under the Coxeter-Weyl group $W(a_n)$ are the Delone polytopes and tile the root lattice in an alternating manner [1-2]. $W(a_n)\,(\omega_1) + W(a_n)\,(\omega_n), W(a_n)\,(\omega_2) + W(a_n)\,(\omega_{n-1}), \dots$ A convenient set of vectors with n components $k_i = \sqrt{\frac{2}{n+1}}\left(\cos\left(\frac{2\pi i}{n+1}\right), \sin\left(\frac{2\pi i}{n+1}\right), \cos\left(\frac{4\pi i}{n+1}\right), \sin\left(\frac{4\pi i}{n+1}\right), \dots\right), (i = 1,2,\dots,n+1)$ (for even n) are introduced where the roots are given by $\alpha_i = k_i - k_j, (i \neq j = 1,2,\dots,n+1)$. For odd n one more component $\frac{(-1)^i}{\sqrt{2}}$ is required. They are useful as the point symmetry $W(a_n) \approx S_{n+1}$ of the lattice permutes the vectors k_i, the first two components of which define the Coxeter plane. The weight vectors can be expressed as $\omega_i = k_1 + k_2 + \cdots + k_i$. The 2D faces of the Delone polytopes tiling the root lattice are equilateral triangles but the projected tiles are the right angle isosceles triangle for $n = 3$, Robinson triangles for $n = 4$ and Danzer triangles for $n = 6$ and so on [3].

Delone cells of the weight lattice A_n^* are copies of the fundamental simplexes whose vertices are defined as $0, \omega_1, \omega_2, \dots, \omega_n$. Although the 2D faces of the fundamental simplex in n-dimensions are not equilateral triangles their projected tiles are exactly the same class of triangles as those of the tiles obtained from the projection of the lattice A_n.

An analysis of the Voronoi cells of both lattices has been worked out in terms of the vectors k_i. The vertices of the Voronoi cell $V(0)$ of the root lattice A_n is the union of the orbits $W(a_n)(\omega_1 \cup \omega_2 \cup \dots \cup \omega_n)$ and the 2D faces are the rhombuses. The Voronoi cell $V(0)^*$ of the weight lattice A_n^* is a permutohedron of degree n and its vertices are the permutations of the vectors k_i of the vertex $\frac{1}{n+1}[(n+1)k_1 + nk_2 + \cdots + k_{n+1}]$. It has regular hexagons and squares as the 2D faces.

Projections of the 2D faces of the Voronoi cells of the root and weight lattices are studied. The tiles obtained from the Voronoi cell projection of the lattice A_4 are the thin and thick Penrose tiles. The projected tiles from the Voronoi cell of the lattice A_4^* are also obtained that leads to a different tiling scheme which has not been studied earlier [4].

The list of tiles and some patches obtained by the tiles are illustrated in the text.

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Theoretical studies of an artificial spin ice on the Ammann-Beenker tiling

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Artificial spin ices (ASIs) consist of nanomagnets decorated on geometric lattices, and topological frustration in these systems often results in interesting and emergent behaviour [1]. While an extensive variety of periodic geometries have been explored, few aperiodic structures have been studied as ASIs [2][3]. Motivated to broaden the scope of aperiodic ASIs, we investigate the magnetic properties of an Ammann-Beenker tiling ASI.

We use a simple Metropolis Monte Carlo algorithm to simulate a system of ~2400 spins, employing a dipolar Hamiltonian with an enhanced Ising term for nearest-neighbour interaction. As we cool down through 180 temperatures, we sample the energy and magnetisation to calculate the specific heat and magnetic susceptibility of our system. To complement this approach, we employ micromagnetic simulations to identify the energies of the ground and excited states of individual vertices.

Using this approach, we observe an anti-ferromagnetic ground state following a transition from paramagnetic disorder. We find that the 8-spin vertices reach their lowest energy configuration at higher temperatures compared to the other vertex types and remain unchanged throughout the remaining quench. On the other hand, 5-spin vertices lie in excited states with energies very close to their ground. We also observe finite magnetic charges and study their magnitude and distribution.

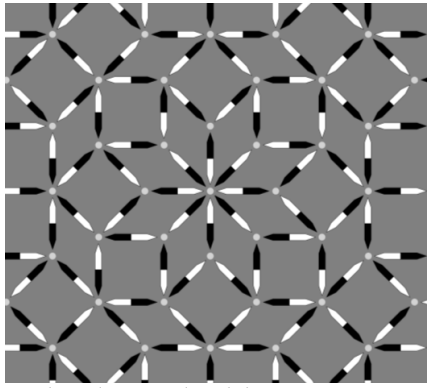

Figure 1 Ammann-Beenker tiling decorated with bar nanomagnets, as indicated by ellipsoids with black and white poles. Vertices are highlighted by circles.

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Non-ergodic states in icosahedral quasicrystals Zn-Mg-*RE* (*RE* = Tm, Er, Ho)

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The magnetism of icosahedral quasicrystals (*i*-QCs) has been studied mainly on Tsai-type QCs, due to the discovery of the $Cd_{5.7}Yb$ *i*-QC and its high-quality structural model. Research on other types of *i*-QCs has been more or less neglected. Studies have shown that all magnetic QCs exhibit spin-glass-like freezing behavior. An exception is the discovery of the first ferromagnetic QCs in the Au-Ga-Gd and Au-Ga-Tb systems [1]. In this contribution, we present a study on the magnetism of *i*-QCs in the Zn-Mg-*RE* (*RE* = Tm, Er, Ho) system with Bergman-type structures. This type of *i*-QCs crystallize into primitive (P) and face-centered (F) phases. Single crystals approximately 1 mm in size were grown using the self-flux method, and all samples have well-defined faces (Fig. 1). Scanning electron microscopy (SEM) and EDS elemental mapping confirmed that the samples are of high quality, with minimal precipitates. Measurements of temperature-dependent zero-field-cooled (zfc) and field-cooled (fc) magnetizations show paramagnetic behavior down to ~1 K. Below 1 K, a splitting appears between M_{fc} and M_{zfc}, with M_{zfc} exhibiting a cusp. Additionally, a peak appears in the specific heat, which broadens and shifts with increasing external field. These observations are characteristic of a non-ergodic spin system and indicate the formation of a spin-glass phase [2].

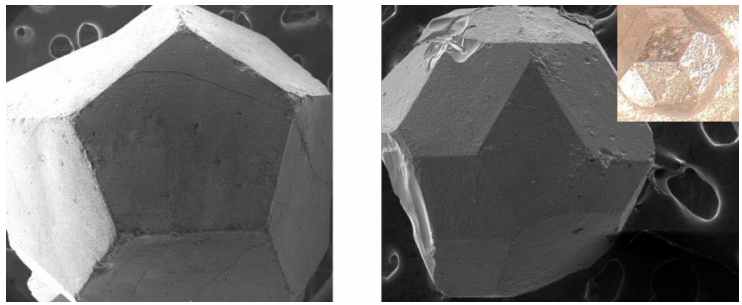

Fig.1: The SEM images reveal well-defined, regular shapes of the investigated *i*-QC. Left panel: Zn-Mg-Ho F-type with pentagonal faces; right panel: Zn-Mg-Ho P-type with rhombic faces (inset: optical microscope image).

Acknowledgements: The Slovenian authors acknowledge the financial support from the Slovenian Research and Innovation Agency (Research Core Funding No. P1-0125 and Project No. N1-0330).

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Single electrons on the Fibonacci quasicrystal: an interpolation between models

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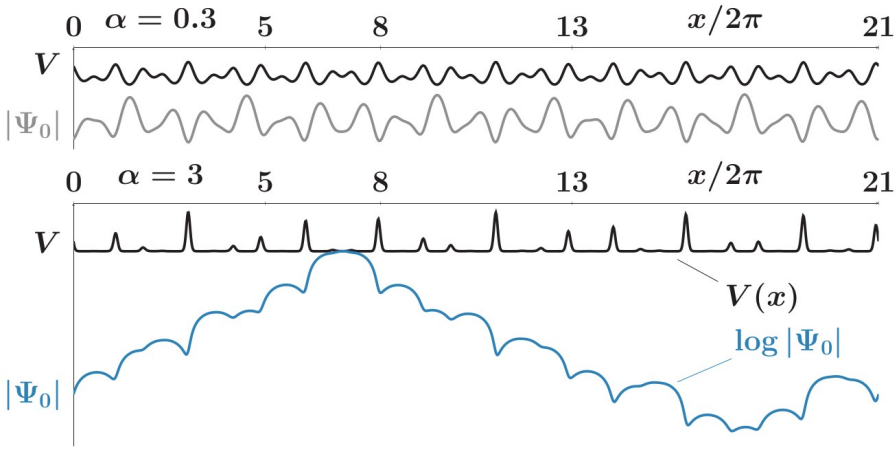
Quasicrystals are some of nature's most intriguing, and quite surprising, forms of matter. They are not periodic in space, nevertheless their constituent atoms and molecules are well-ordered in space. Here, we discuss the theory for the eigenstates and spectral properties of the equation for single electrons in a quasicrystal. Bloch theory is the theory that governs eigenstates (the electronic wavefunction in quantum mechanics) in spatially periodic crystals, and is a cornerstone theory for understanding how electrons behave in periodic crystals. There is as yet no comparable theory for electrons in aperiodic crystals, and this is an area where mathematical and physical insight need to be combined. Three kinds of eigenstates are known: eigenstates for electrons that extend across the whole crystal, eigenstates that are exponentially localised in space, representing electrons that are caught by the aperiodic nature of the quasicrystal, and a third intermediate state with algebraic decay in space. We investigate this behaviour in a one-dimensional aperiodic crystal based on the so-called Fibonacci tiling. We solve the problem numerically using both periodic approximants and a two-dimensional projection method. We use a new model that interpolates between representing atoms as a smoothly varying potential function and representing atoms as delta functions. Real atoms in real crystals are best described by something in between these limits, and our interpolating model allows two (and possibly all three) kinds of eigenstates, helping us understand how they are related.

Acknowledgements: We are grateful for support from the Leeds Cheney Fellowships Scheme and from the Israel Science Foundation (ISF) grant 1259/22.



Synthesis and thermoelectric properties evaluation of Al-Ge-Ru 1/0 approximant crystals

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In 2019, the world's first semiconducting approximant crystal (AC) was discovered in the Al–Si–Ru system by Iwasaki *et al.* [1]. This AC exhibits a low thermal conductivity (κ) of 1.5 W m^{-1} K^{-1} and a high Seebeck coefficient (S) of 200 μV K^{-1} at 350 K comparable to practical thermoelectric materials, suggesting the potential of semiconducting ACs for thermoelectric applications. However, the low electrical conductivity (σ) of 30 S cm^{-1} at the same temperature has been a bottleneck in achieving high thermoelectric performance, and further improvement in thermoelectric properties through doping has been attempted [2]. Meanwhile, no studies have discovered new semiconducting AC in other systems, and their thermoelectric properties remain much unexplored. This study is designed to synthesize new semiconducting ACs in the related compounds, the Al–Ge–Ru system, and investigate their thermoelectric properties.

Polycrystalline Al–Ge–Ru ACs were prepared by arc-melting and annealed at 1273 K for 1 week under Ar atmosphere. The resulting samples were sintered using the spark plasma sintering method, followed by annealing at 1273 K for 1 week under Ar atmosphere. The phase purity of the samples was examined by powder X-ray diffraction using CuKα radiation and SEM-EDS elemental analysis. σ and S were measured under He atmosphere between 300 and 873 K using the four-probe method and the steady-state temperature gradient method, respectively. κ was measured using the laser flash method in the temperature range of 300 − 873 K.

Phase analysis confirms that the synthesized samples are in a single-phase 1/0 AC in the Al–Ge–Ru system. The Al–Ge–Ru 1/0 AC, like the Al–Si–Ru 1/0 AC, exhibits a low κ of 1.0 − 1.5 W m^{-1} K^{-1} and a high S of −200 μV K^{-1} at 300 K, though the sign of S is opposite. Notably, the magnitude of σ of the present system (270 − 690 S cm^{-1}) is about 9 − 30 times higher than that of Al–Si–Ru 1/0 AC at 300 K, resulting in a maximum figure of merit (zT) of 0.28 at 473 K, which is the highest value ever reported thus far among quasicrystals and ACs exhibiting negative S. In this presentation, we will discuss the thermoelectric properties of the Al–Ge–Ru 1/0 AC, focusing on their temperature and compositional dependencies.

Acknowledgements: This work was supported by JSPS KAKENHI Grant Numbers JP19H05817 and JP19H05818, and by JST CREST Grant Number JPMJCR22O3.

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Physical properties of supersilent high-entropy alloys

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Searching for materials that possess a combination of excellent magnetic softness and vanishing magnetostriction, the ferromagnetic high-entropy alloy (HEA) systems $AlCoFeNiCu_x$ (x = 0.6–3.0) and $(GaNi)_xCoCrFe$ (x = 0.4–1.6) were investigated. We have characterized structure, microstructure, nanostructure and chemical composition of the individual phases in the multi-phase alloys and determined their magnetic, magnetostrictive and electrical properties. We found that the alloys are ferromagnetic and exhibit functional combination of magnetic softness and vanishing magnetostriction, classifying them as energy-efficient "supersilent" materials (inaudible to a human ear) for alternating-current (AC) electromagnetic applications in the audio-frequency range.

In the copper (Cu) series we obtained superior parameters for the composition $AlCoFeNiCu_{2.0}$, which shows zero magnetostriction, $\lambda_s = 0$, low coercivity $H_c \approx 650$ Am^{-1} and substantial saturation magnetic polarization of $J_s \approx 0.55$ T. The parameters of other $AlCoFeNiCu_x$ compositions in the range x = 2.0–3.0 are only slightly different, so that the entire set of the $AlCoFeNiCu_x$ HEAs in that Cu content range can be classified as magnetically soft and vanishing-magnetostriction alloys [1].

Meanwhile, for the $(GaNi)_xCoCrFe$ series, we obtained superior parameters for the compositions x = 1.3 and 1.6. Magnetic softness and magnetostriction parameters of the x = 1.6 alloy (saturation magnetic polarization J_s = 0.55 T, coercive field $H_c \approx 400$ Am^{-1}, Curie temperature T_C = 700 K, saturation magnetostriction coefficient $\lambda_s = -3$ μmm^{-1} and high RT electrical resistivity ρ_{300K} = 110 μΩcm) are about the same as those of the $AlCoFeNiCu_{2.0}$ alloy, the first reported supersilent HEA. The parameters of the composition x = 1.3 are only insignificantly different [2].

Regarding the microscopic origin of the smart combination of magnetic softness and vanishing magnetostriction, there emerges a question whether these two systems are identical, so that $(GaNi)_xCoCrFe$ is just another variant of the $AlCoFeNiCu_x$, or there are some fundamental physical differences between them. The origin of magnetic softness, which is the phenomenon of exchange averaging of magnetic anisotropy, is the same for both systems, while the origin of vanishing magnetostriction is different. In the $AlCoFeNiCu_x$, it is a result of compensation of magnetostrictions of opposite signs of the two present ferromagnetic phases, whereas in the $(GaNi)_xCoCrFe$, it originates from the nanostructured morphology of a single ferromagnetic phase. There thus exists a fundamental difference between the $AlCoFeNiCu_x$ and the $(GaNi)_xCoCrFe$ multi-phase HEA systems.

Acknowledgements: The Slovenian authors acknowledge the financial support from the Slovenian Research and Innovation Agency (Research Core Funding No. P1-0125 and Project No. N1-0330).

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A Julia Software Suite for Crystallography in Arbitrary Dimensions

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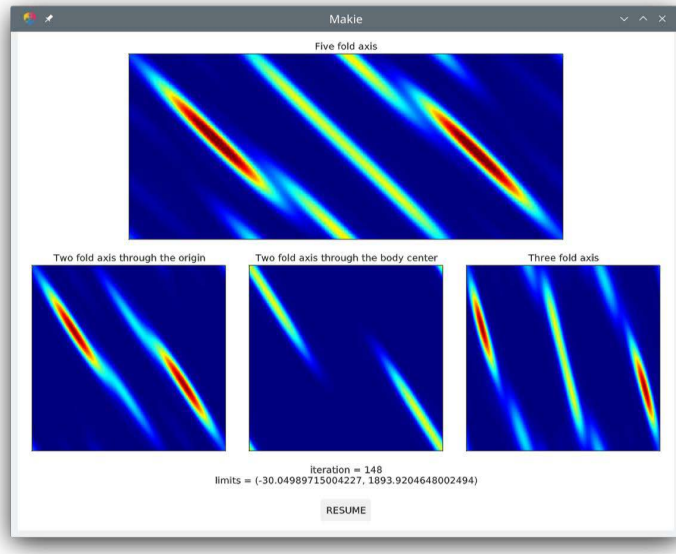
We present a software suite for crystallographic computations with an emphasis on quasicrystals. The suite comprises two Julia packages: **SpaceGroups** [1] and **ChargeFlipPhaser** [2].

SpaceGroups provides a general framework for defining and manipulating space groups in spaces of arbitrary dimension. Users can define space groups via their generators and specify special Wyckoff positions, with automatic validity verification. The package also supports reciprocal-space analysis, identifying Bragg peak types—real, complex, or extinct—based on space group symmetries.

ChargeFlipPhaser implements a generalized charge-flipping algorithm capable of handling structures with arbitrary space group symmetries. It introduces a symmetry-breaking sampling scheme that both minimizes redundancy and optimizes FFT performance. The package offers fine-grained control over the phasing process via user-defined callbacks and includes a GUI example demonstrating progress tracking and interactive capabilities.

[1] https://github.com/pkfrance/SpaceGroups.jl
[2] https://github.com/pavel-kalouguine/ChargeFlipPhaser.jl



Synthesis and structure analysis of ZnMgEr P-type quasicrystal

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In this presentation we report a synthesis and structure refinement of the new samples ZnMgEr in P-type Bergman type icosahedral quasicrystal family. The synthesis was performed using a self-flux method obtaining single crystal grains of millimeter-size. Selected samples were measured by the single crystal X-ray diffraction resulting in approx. 2500 peaks ($|F|<u(|F|)$). The final structure model was refined against the diffraction data with lowest R-factor of 14% (see Fig. 1). The number of parameters was less than 350. Compared to previously studied structure of $Zn_{70}Mg_{20}Tm_{10}$ [1] the structure model was significantly constrained (with much lower number of free parameters) due to low quality of diffraction data. The future work will be focused on improving the quality of the measurement result and finer structure model allowing for detailed analysis of the influence on the potential physical properties, like magnetism.

Acknowledgements: The work was supported by the Polish National Science Centre under grant no. 2022/47/I/ST3/00340.

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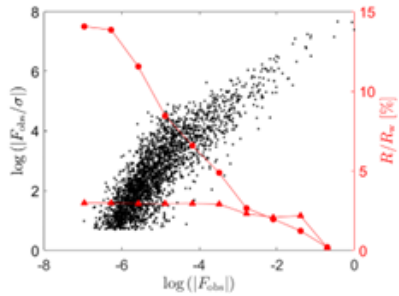

Fig.1: The agreement between experimental and calculated diffraction amplitudes.

Vertex environments in the extended canonical cell tiling

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It is widely recognized that icosahedral clusters in icosahedral quasicrystals and their periodic approximants are interconnected through two types of linkages aligned with the 2-fold and 3-fold symmetry axes. The cluster networks are often described using a geometrical framework based on four types of polyhedra (A, B, C, D in Fig. 1), with edges corresponding to the two types of linkages. This framework, known as the canonical-cell tiling (CCT) [1], facilitates the description of highly efficient cluster packing and has been successful in describing actual periodic approximants [2-5]. However, it has been suggested that certain types of periodic approximants, as well as icosahedral quasicrystals, may not be adequately described within this framework because it does not accommodate local configurations with perfect icosahedral symmetry.

We have therefore proposed an extension of the CCT by introducing two additional types of polyhedra as the prototiles (H and I in Fig. 1). This extended CCT allows for a more flexible representation of various cluster arrangements and enables the description of local configurations with icosahedral symmetry using the icosahedron (I). From geometrical considerations, we have so far been able to deduce some basic properties of the extended CCT. These include general sum rules for the frequencies of the six cells, along with all possible kinds of vertex environments allowed in the extended CCT. In this poster presentation, we will illustrate these findings using color images of all the 197 types of vertex environments as well as a few selected periodic examples, accompanied by simple explanations.

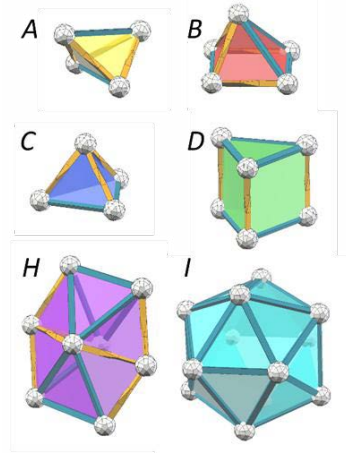

Fig.1: The six prototiles of the extended canonical cell tiling.

Acknowledgements: Financial support from Japan Science and Technology Agency through CREST (Grant no. JPMJCR22O3) is gratefully acknowledged.

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Pd-doped $Al_{13}Fe_4$ as an efficient catalyst for the semi-hydrogenation reaction of acetylene

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The catalytic potential of complex intermetallic compounds, $Al_{13}Fe_4$ and $Al_{13}Co_4$, which are known as periodic approximants to decagonal quasicrystals, for the selective hydrogenation of alkenes and alkynes has been attracting attention [1-6]. It has also been suggested [7] that these compounds can also serve as platforms for creating *single-atom catalysts*, where catalytically active elements are monoatomically dispersed on the surface, potentially leading to much enhanced catalytic performance compared to the platforms themselves. The aim of this study is to clarify the effects of doping Pd into $Al_{13}Fe_4$ on the catalytic activity for the semi-hydrogenation reaction of acetylene ($C_2H_2+H_2 \rightarrow C_2H_4$). We base our experimental investigations on alloy samples with nominal compositions of $Al_{76.5}Fe_{23.5-x}Pd_x$ (x = 0—10), prepared using arc melting, followed by an annealing at 800 °C for 48 hours. These samples are pulverized and sieved to a particle size range of 25—75 μm in diameter before conducting catalytic tests.

The catalytic activity for the semi-hydrogenation reaction of acetylene was assessed using a reaction gas mixture of 2% C_2H_2, 80% H_2, and 18% Argon, with a flow rate of 30 ml/min. The conversion rate, reaction rate, and ethylene selectivity were evaluated from room temperature up to 300 °C. We observed a dramatic increase in catalytic activity as soon as Pd was doped at 1 at%, and the level of activity remained high up to 4 at% Pd. This follows simultaneously a structural phase transition from the monoclinic M-$Al_{13}Fe_4$ to orthorhombic O-$Al_{13}(Fe,Pd)_4$ [8,9] as confirmed by powder X-ray diffraction. Further increasing the Pd content from 5 to 10 at% resulted in an abrupt decrease in activity at temperatures higher than 200 °C, which seems to be due to a higher proportion of the secondary ε-phase that has low degradation resistance. The ethylene selectivity remained high (~90 % at 200—300 °C) for all our samples. Furthermore, we performed first-principles calculations to elaborate on the site selectivity of Pd atoms in the crystal structures as well as the structural transition. We find that Pd atoms substitute specific Fe sites in both monoclinic and orthorhombic phases, creating specific local configurations around dispersed Pd atoms, which may be associated with the enhancement in catalytic activity.

Acknowledgements: This work is financially supported through the CREST program (Japan Science and Technology Agency, Grant no. JPMJCR22O3) and the Tohoku University-Université de Lorraine Joint Research Fund 2024.

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Structural investigation of the Ho-Au-Si(100) approximant surface

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The discovery of Quasicrystals (QC) in 1982 by Dan Schechtman has generated a huge interest because of their unique structures and properties. Lacking periodicity in 3-dimensional space, quasicrystals have an atomic arrangement described by the assembly of highly symmetric atomic clusters. For each quasicrystal corresponds one or more quasicrystalline approximants. The latter crystals exhibit building blocks similar to those identified in the QC and present this time a translationnal symmetry. The Au-Si-RE (Rare-Earth) quasicrystalline approximants have a structure close to the $MCd_{5.7}$ (M=Ca, Yb) quasicrystal built from Tsai-type clusters. These quasicrystalline approximants have been identified for their remarkable magnetic and thermoelectric properties derived from their complex structure [1]. A Tsai-type cluster has concentric shells consisting of a tetrahedron at its center followed by a dodecahedron, an icosahedron, an icosidodecahedron and a rhombic triacontahedron.
Unlike the bulk, the atomic structure and surface properties of these Au-Si-RE approximants remain unexplored. Several key questions await answers, including the stability of the clusters once exposed to the surface [2]. Here we propose a characterization of the (100) surface of the Tsai-type approximant $Ho_{1.04}Au_{4.85}Si_{1.324}$ using both experimental techniques and density functional theory (DFT). Low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) show a (2x1) surface reconstruction. The patterns present on the surface are comparable to the patterns present on one of the bulk planes for which DFT calculations were performed. The ultraviolet photoemission spectroscopy measurements and the bulk calculation of the electronic density of states show that the valence band is dominated by Au 5d states. The reactivity of this surface was studied by oxygen and C_{60} adsorption. After oxidation, the X-ray photoelectron spectroscopy measurements show a segregation of Si and Ho at the surface induced by oxygen adsorption. The deposition of a thin film of C_{60} molecules lead to a c(2x2) type superstructure. The highest symmetry matching between the C_{60} molecule and the surface is obtained when a pentagonal face of the C_{60} molecule is facing the surface at specific surface atomic sites.

Acknowledgements: This work was supported by the European C-MAC consortium. The authors thank GENCI for the access on national HPC resources of (IDRIS, TGCC, CINES). They also thank the EXPLOR center hosted by the Université de Lorraine for CPU time and assistance. E.G. acknowledges financial support through the COMETE project cofunded by the European Union under the program FEDER-FSE Lorraine et Massif des Vosges. This work was supported by the Knut and Alice Wallenberg Foundation (grant number KAW 2018.0019).

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Surface structure of Nd-Fe-B permanent magnets.

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Rare-earth (RE)-based permanent magnets, such as Nd-Fe-B, are essential materials for Europe's energy future, playing a key role in the construction of motors for electric vehicles and wind turbines, among other applications. These materials exhibit exceptional magnetic properties, which are based on the $Nd_2Fe_{14}B$ phase. The latter features a high saturation magnetization, a strong uniaxial magnetocrystalline anisotropy responsible for a significant remanence (Br), and a high intrinsic coercivity (H_{ci}), making it resistant to demagnetization. However, Nd-Fe-B magnets are complex, multiphase materials [1], whose properties are not solely dictated by the intrinsic characteristics of the $Nd_2Fe_{14}B$ phase but also by the overall microstructure of the material, particularly the nature of the intergranular phases formed during the processing stage. In conventionally sintered magnets, $Nd_2Fe_{14}B$ grains are microscopic, and intergranular phases form at grain boundaries. When the material is subjected to a demagnetizing field, the demagnetization process initiates at interfacial regions, which may exhibit lower coercivity, and then rapidly propagates (nucleation model). The coercivity is strongly influenced by the chemical, structural, and magnetic properties of the intergranular phases. Despite all the progress made so far, the coercivities observed in Nd-Fe-B permanent magnets account for only 20% of the theoretically achievable value (i.e., H_a), indicating that significant improvements are still possible. In this context, one approach is to develop Nd-Fe-B permanent magnets composed of $Nd_2Fe_{14}B$ grains free from intergranular phases and parasitic impurities while recreating new, in-situ controlled interfaces using novel processing techniques.

In this work, the objective is to create model interfaces using $Nd_2Fe_{14}B$ single crystals as substrates, onto which previously optimized, intergranular phase thin films will be deposited and thoroughly characterized. To achieve this, high-structural-quality $Nd_2Fe_{14}B$ single crystals are grown using a flux method. The first challenge is to optimize the preparation conditions of $Nd_2Fe_{14}B(001)$ surfaces and to characterize them under ultrahigh vacuum. Low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) reveal that the surface exhibits a c(2×2)-type reconstruction with a terrace and step morphology separated by a unique step height. This indicates that a specific bulk plane is selected as the surface layer. X-ray photoelectron spectroscopy (XPS) analysis shows the presence of neodymium oxide, which progressively disappears with successive preparation cycles.

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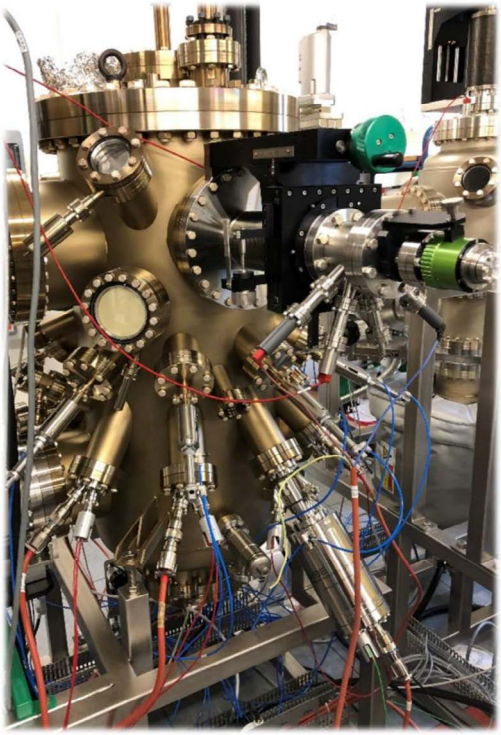

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