MS25-P2 Brick tiling

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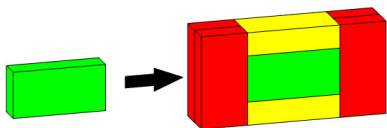

Figure 1. Three-dimensional brick inflation.

Keywords: brick tiling, lattice substitution tiling

MS25-P3 First surface structure determination of a quasicrystalline approximant using combined surface x-ray diffraction and ab initio calculations.

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

In this work, we re-investigate the pseudo-10fold surface of the $Al_{13}Co_4$ complex intermetallic compound (Fig. 1 left) [1,2], considered as a decagonal approximant, using both surface x-ray diffraction (SXRD) and density functional theory (DFT) calculations. SXRD has the advantage compared to dynamical low-energy electron diffraction (LEED-IV) that one can generally ignore multiple scattering, which makes data analysis more straight-forward. The determination of the surface structure by SXRD was only possible due to the large experimental dataset which could be recorded at ESRF – the largest experimental dataset ever analyzed with this technique – a consequence of the high density of crystal truncation rods and of the relatively low symmetry of the system.

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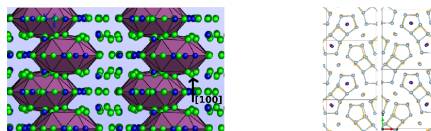

Figure 1. *Left: Crystal structure of $Al_{13}Co_4$ highlighting Henley-type clusters. Right: Comparison of positions of surface atoms deduced from SXRD (blue) and DFT (red-orange).*

MS25-P4 A complex pseudo-decagonal quasicrystal approximant solved by the strong reflections approach and refined against Rotation Electron Diffraction (RED) data

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The strong-reflections approach is valid on structures that contain similar atomic clusters and electron diffraction patterns with similar intensity distribution of reflections. It is based on the fact that the strongest reflections largely determine the atomic positions in a structure and represent the main structure features of a crystal. Thus, this approach can be used for structure solution. In the present study, the structure of the complex pseudo-decagonal (PD) quasicrystal approximant PD1 in the Al-Co-Ni alloy system was solved by phasing the strong reflections from rotation electron diffraction [1] (RED) data using the known PD2 structure [2]. The PD1 crystal is primitive and orthorhombic $Pnam$, with unit cell parameters a=37.7, b=39.7, c=4.1 Å. Electron diffraction studies show that in reciprocal space, the positions of the strongest reflections and their intensity distributions are similar for both approximants. The high-resolution transmission electron microscopy (HRTEM) image after image processing with CRISP (crystallographic image processing program) shows that PD1 and PD2 intergrow with each other. The orientation relationship between PD1 and PD2 was found by comparing the Fourier transforms, calculated from the two regions in the HRTEM image. By applying the strong-reflections approach, the structure factor amplitudes and phases of PD1 were deduced from those of the known PD2 structure. The structure of PD1 contains 115 unique atoms (31 Co/Ni and 84 Al). They were located from a density map calculated from only the 15 (!) strongest unique reflections. As with other approximants in the PD series, PD1 is built of characteristic 2 nm wheel clusters with 5-fold rotational symmetry [3], which agrees with results from HRTEM images.

References

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