

**MS25-P2** Brick tilingShelomo I. Ben-Abraham<sup>1</sup>, Dvir Flom<sup>1</sup>

1. Department of Physics, Ben-Gurion University of the Negev, POB 653, IL-8410501 Beer-Sheba, Israel

email: shelomo.benabraham@gmail.com

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  $2^{(d-1)} d! = 2^{2 \times 3/2} = 2^3 = 8$  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  $6 \times 8 = 48$  "colors" and constructed a lattice substitution tiling that reproduces the brick tiling. We also discuss possible generalizations to arbitrary dimensions.

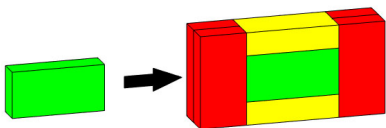


Figure 1. Three-dimensional brick inflation.

**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.

Emilie Gaudry<sup>1</sup>, Corentin Chatelier<sup>1</sup>, Roberto Felici<sup>2,3</sup>, Jakub Drnec<sup>2</sup>, Marc de Boissieu<sup>4,5</sup>, Guillaume Beutier<sup>4,5</sup>, Laura Serkovic Loh<sup>1</sup>, Garry McGuirk<sup>1</sup>, Marie-Cécile de Weerd<sup>1</sup>, Julian Ledieu<sup>1</sup>, Vincent Fourné<sup>1</sup>

1. Institut Jean Lamour - Université de Lorraine CMRS UMR 7198
2. ESRF, Grenoble, France
3. CNR-SPIN, Area della ricerca di Tor Vergata, Via del fosso del cavaliere 100, Roma, Italy
4. Université Grenoble Alpes, Simap, Grenoble, France
5. CNRS Simap, Grenoble, France

email: emilie.gaudry@univ-lorraine.fr

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 – as 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  $1.09 \text{ J/m}^2$ . 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.

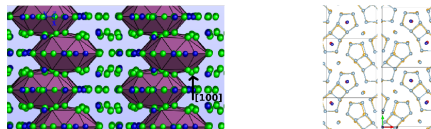


Figure 1. Left: Crystal structure of  $Al_{13}Co_4$  highlighting Henley-type clusters. Right: Comparison of positions of surface atoms deduced from SXRD (blue) and DFT (red-orange).