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To cite this version:

HAL Id: jpa-00212430
https://hal.archives-ouvertes.fr/jpa-00212430
Submitted on 1 Jan 1990

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Short Communication

A quasi-crystalline sphere-packing with unexpected high density

Jörg M. Wills


(Reçu le 23 janvier 1990, accepté sous forme définitive le 5 mars 1990)

Résumé. — Henley, puis Olamy et Kléman ont construit des pavages de Penrose à 2D par empilements de disques de grande densité. A l'aide de ces empilements, on a construit un pavage de Penrose à 3D par empilement de sphères d'une densité de 0,67798, plus élevée que la meilleure densité connue pour les quasicristaux usuels. Cet empilement pourrait fournir un modèle de quasicristaux cylindriques, récemment découverts par Bendersky et al., Schaefer et al. et Fung et al.

Abstract. — Hendley and later Olamy and Kléman constructed circle packings in 2D-Penrose tilings of high packing densities. From these circle packings one obtains with an additional idea a sphere packing in a cylindrical 3D-Penrose tiling of packing density 0.67798..., which is higher than the best known packing densities of 0.62... for usual quasicrystals. This packing might be a model for the cylindrical quasicrystals discovered by Bendersky et al., Schaefer et al. and Fung et al.

1. Introduction.

Atomic dense packing is a fundamental property of condensed matter. So recently several authors have investigated dense sphere packings in quasicrystalline structures, e.g. Henley [1], Olamy and Alexander [2], Olamy and Kléman [3], and Oguey and Duneau [4]. Moreover, Henley and Olamy and Kléman investigated dense circle packings in 2D-Penrose tilings. In this paper we construct cylindrical sphere packings based on these 2D-Penrose tilings; i.e. our two basic rhombohedra are not the usual golden or Ammann-rhombohedra, but they are orthogonal prisms over the two Penrose rhombs. Because of their high density these packings might be interesting from the structural viewpoint. Quasicrystals of cylindrical type, i.e. with one translation axis were discovered in 1985 by Bendersky et al. [5], Schaefer et al. [6] and Fung et al. [7]; so our sphere packing might be a model for quasicrystals of this type.

2. Construction.

For our 3D-tiling we need the 2D-tiling which is described in detail in Olamy and Kléman (pp. 28, 29). So to save space we use their terminology and results. As Olamy and Kléman point out
(p. 29) their "matching rules" are no "forcing rules", i.e. they do not enforce quasiperiodicity. So "packing rules" might be more appropriate. But we use "matching rules" further on in accordance with the Olamy-Kléman-terminology. We mention further that Henley's matching rules [1] work as well, but they lead to slightly smaller densities.

The construction: to fix a scale we consider only unit spheres, i.e. of radius 1. Then the two basic rhombohedra have edge-length $\sqrt{3}$ and height 2.

The fat rhombohedron has basic angles of 72° and 108°; the thin rhombohedron has basic angles of 36° and 144°. Five of the fat rhombohedra generate a 5-star-prism $\Sigma$ of height 2 (see Fig. 1); three fat rhombohedra and one thin rhombohedron generate a diamond-prism $\Delta$ of height 2 and one fat rhombohedron together with two thin rhombohedra generate a hexagonal prism $H$ of height 2 (see Fig. 2). Elementary calculation shows for the volumes of the thin rhombohedron:

$$V = 6 \sin 36$$

and for the fat rhombohedron:

$$V = 6\tau \sin 36, \text{ where } \tau = \frac{1}{2} \left(\sqrt{5} + 1\right).$$

So one gets for the volume of the prisms $\Sigma, \Delta$ and $H$:

$$V_{\Sigma} = 30\tau \sin 36, \quad V_{\Delta} = 6(3\tau + 1) \sin 36, \quad V_H = 6(\tau + 2) \sin 36.$$
The average volume of the sphere packing is
\[ \frac{4}{3} \pi (n_\Sigma + n_\Delta + n_H) = \frac{4}{3} \pi (3 \tau - 2). \]

The average volume of the prisms \( \Sigma, \Delta \) and \( H \) is
\[ V_\Sigma + V_\Delta + V_H = 6 \sin 36 (5 \tau^{-2} + (3 \tau + 1) \tau^{-4} + (\tau + 2) \tau^{-1}) = 30 \sin 36. \]

So one obtains for the density
\[ \delta = \frac{4}{3} \pi (3 \tau - 2) \cdot (30 \sin 36)^{-1} = 0.67798... \]

Until now we have an infinite slice of height 2 endowed with a 2D-Penrose tiling. If we take infinitely many congruent copies of this slice and fit them together such that in the vertical direction the whole packing is invariant under translations of length 2, we obtain the desired cylindrical 3D Penrose packing. Of course, this packing has the same density
\[ \delta = 0.67798... \]

which is much higher than the best known densities in quasicrystals generated by the Ammann-rhombohedra (with \( \delta = 0.62... \)). Moreover this packing is stable, i.e. no sphere can be moved essentially from its position without touching another sphere.

References