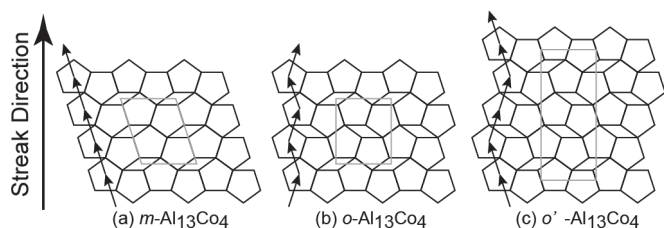


On the basis of careful examinations of diffraction peak appearances, we find a striking feature that the stacking periods are extended into extremely long distances, typically being longer than $\sim 100\text{\AA}$. Furthermore, even though there are many stacking sequences possible for a given periodic length, each of the observed stacking structures can be uniquely determined according to the polytype series generated by a hyperspace crystallography, as combined with a systematic introduction of shear strains for a hyper-cubic crystal. This intriguing fact in turn implies that the occurrence of the present long-period variants is restricted by the hidden order along the hyperspace dimension. For understanding an origin of this restriction in terms of temperature dependence of the length-scale change, we applied axial next-nearest-neighbour ising model to the present polytype structures, by defining the stacking direction parameters with an analogy of up-down spin configurations. According to the Monte Carlo simulations, we are able to reproduce the intense peak shift depending on temperature. This suggests that the second nearest-neighbour interactions play a critical role for realizing the extremely long-period order and perhaps incommensurate aperiodic order.



[1] T. Gödecke et al., *Z. Metallkde.* **1996**, *87*, 854. [2] B. Gruschko et al., *J. Alloys and Comp.* **1996**, *233*, 279. [3] F. Fleischer et al., *J. Alloys and Comp.* **2010**, *500*, 153.

Keywords: quasicrystal, polytype, incommensurate

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Application of average unit cell concept to 3D Amman-kramer tiling

Radosław Strzałka, Bartłomiej Kozakowski, Paweł Kuczera, Janusz Wolny, *Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Kraków (Poland)* E-mail: radek.strzalka@gmail.com

Amman-Kramer tiling is a 3D generalization of the Penrose tiling. It consists of two kinds of structure units: prolate and oblate rhombohedra with all edge lengths equal. All faces of the structure units are identical rhombuses. The ratio of the face diagonals is equal to τ , and the acute angle amounts to $\arctan(2) = 63.44^\circ$. The volume ratio of the unit tiles as well as the ratio of their frequencies in the tiling also equals τ . Amman-Kramer tiling reveals an icosahedral symmetry, thus it can be used as a quasilattice for building a model of an icosahedral quasicrystal.

One can generate the set of points of the Amman-Kramer tiling by projecting a 6D hypercubic lattice via 3D window – the so called atomic surface. In case of the tiling the atomic surface has the shape of a rhombic triacontahedron (Fig.1).

We present a derivation of the structure factor of the Amman-Kramer tiling on the basis of the average unit cell concept [1], which allows a structure factor calculation in physical space only. This method has been successfully used to perform a structure refinement of the decagonal basic Ni-rich Al-Ni-Co phase [2,3].

Any point of the tiling can be written in the so called reference

lattice: $r_i = n_i \lambda_i + u_i$, $\lambda_i = 2\pi/k_i$, where: $i=x,y,z$, n_i is an integer, λ_i is a reference lattice constant for a given direction and u_i is a position in the reference lattice. The reference lattice constant is related to a scattering vector k_i , which is observed in the diffraction pattern. The position distribution of Amman-Kramer tiling points $P(u_x, u_y, u_z)$ is called an average unit cell (Fig.1). Because of the aperiodicity of the tiling the distribution $P(u_x, u_y, u_z)$ should be related to another one $P(v_x, v_y, v_z)$, whose lattice constants are elongated by τ . A 6D distribution $P(u_x, u_y, u_z, v_x, v_y, v_z)$ is only nonzero along lines: $v_i = -\tau^2 u_i$. This is a characteristic feature of quasicrystalline lattices. One can show that there is a linear relation between the shape of the distribution and the shape of the atomic surface. A structure factor for any scattering vector can be calculated as a Fourier transform of this distribution. It is important to see that because of the characteristic relation between v_i and u_i , the Fourier transform actually reduces to a 3D integral.

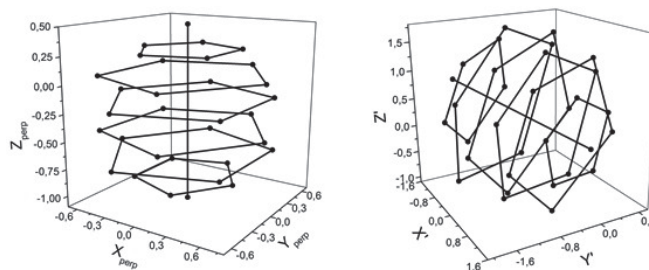


Figure 1. Atomic surface (left) and the average unit cell (right) for Amman-Kramer tiling.

The comparison between structure factors obtained with three methods (numerical calculations, in the perpendicular space and with average unit cell concept) will be presented to show the perfect agreement. The results of first attempts to fit the Cd-Yb [4] experimental data to our model will be discussed.

[1] J. Wolny, *Phil. Mag.* **1998**, *77*, 395-412. [2] J. Wolny, B. Kozakowski, P. Kuczera, H. Takakura, *Z. Kristallogr.* **2008**, *223*, 847-850. [3] P. Kuczera, B. Kozakowski, J. Wolny, W. Steurer, *JPCS* **2010**, *226*, 1-7. [4] H. Takakura, C.P. Gomez, A. Yamamoto, M. De Boissieu, A.P. Tsai, *Nature Materials* **2007**, *6*.

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Multidimensional paperfolding substitution structures

Dekel Shapira,^a Shelomo I. Ben-Abraham,^a Alexander Quandt,^b ^aDepartment of Physics, Ben-Gurion University of the Negev, Beer-Sheba, (Israel). ^bSchool of Physics, University of the Witwatersrand, Wits, (South Africa). E-mail: nopede@gmail.com

We succeeded to generalize the substitution for the regular one-dimensional paperfolding sequence to two and more dimensions enabling us to construct multidimensional paperfolding structures. We elaborate the algorithm in detail. Here we explicitly present a two-dimensional example of the structure. We display the successive generations using the alphabet $\{+, \}$ as well as a “realistic” image of a folded paper sheet. We show the calculated Fourier spectrum which is known to have a dense pure point (Bragg) part. We compute the rectangle complexity which is polynomial and hence the entropy vanishes.

Keywords: paper folding structure, substitution