Re-refinement of AlCuRh decagonal quasicrystal with a quasilattice based on the generalized Penrose tiling

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In structural modeling of decagonal quasicrystals mostly rhombic or pentagonal Penrose tiling are used as quasilattices with a great success. The question arises, whether these types of tilings are "the best" of all other possible tilings from the common Penrose local isomorphism class. Our recent studies are focused on the development of the generalized Penrose tiling in modeling of decagonal systems [1,2]. By introducing a shift along *z*-direction in multidimensional hyperspace, controlled by a single extra parameter, a whole set of new local configurations of structural unit tiles (thick or thin rhombuses) appears, giving an additional room for maneuver during a refinement process. By shifting the 5-dimensional window in hyperspace, an additional pentagonal atomic surface in the perpendicular space appears, and the other 4 atomic surfaces change into non-uniform decagons. The subdivision of atomic surfaces into regions corresponding to a given unit tile at a given orientation hexagonal shapes appear, whereas triangles were observed in the case of the regular, rhombic Penrose tiling. New local arrangement of tiles introduce more freedom in the refinement and, likely, a better overall result can be expected. Our study show the result of structure refinement of AlCuRh decagonal quasicrystal, first investigated by Kuczera *et al* [3]. This system can be treated as representative decagonal quasicrystal with one of the least amount of diffuse scattering observed in the diffraction pattern known, which suggest a highest order in the atomic structure. We constructed a starting model based on the generalized Penrose tiling with starting decoration derived from the phased electron density map obtained from superflip tool, and the synchrotron data collected previously by Kuczera, and performed a refinement. The process converged with R-factor of 6.52%, which is a significant improvement in compare with 7.9% reported in the original paper. The standard correction for phonons and phasons was used. Using only the generalized Penrose quasilattice and keeping atomic positions fixed improved the refinement result by a factor of 0.2%. We checked a particular quasilattice obtained by a shift parameter 0.2. The further studies will be focused on implementing a shift parameter as additional parameter to refine, and to search the "best" type of Penrose tiling for decagonal AlCuRh.

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2. R. Strzałka, I. Buganski, M. Chodyn, J. Wolny, *Sci. Rep.*, submitted.

2. P. Kuczera, J. Wolny, W. Steurer, *Acta Cryst. B*, **68**, (2012), 578-589.