Structure of decagonal quasicrystals described by clusters

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The best fitting structure model of 2D decagonal quasicrystals is the Penrose tiling. It is filled up by two sets of rhombuses, which are arranged non-periodically throughout the space. Atoms put in the vertices of rhombuses produce diffraction pattern with the forbidden, five-fold symmetry - observed in the experimental data of real quasicrystaline samples.

Apart from the rhombus model there are also other ones, which are being intensively developed; like the high-dimensional "cut-and-project" model or the statistical model. However, it is the cluster model which has been the focus of attention, since its discovery. Petra Gummelt, the discoverer of the cluster, proved that only one structure element is needed to cover to whole Penrose tiling. It has but one unique and new property – clusters must overlap each other or, in other words, must share the atoms. This feature results in some restriction in the number of independent atoms, which can decorate the cluster. Gummelt's Cluster – G33 – contains 33 atoms but due to the overlapping rules only 3 of them are independent. Another type of cluster is the kite-cluster. It has some new, distinctive features when compared to G33. It is smaller - thus the overlapping rules are less restricting and more independent atoms can decorate it; and it can be easily down and up-scaled for the best fitting results. Fig. 1 shows 3 types of kite-clusters: K17, K7 and K4 with 17, 7 and 4 atoms, though only 7, 3 and 2 are the independent ones. The relative concentration of atoms filling-up the kite-clusters is similar to the relative concentration of the atoms building the quasicrystaline compounds.

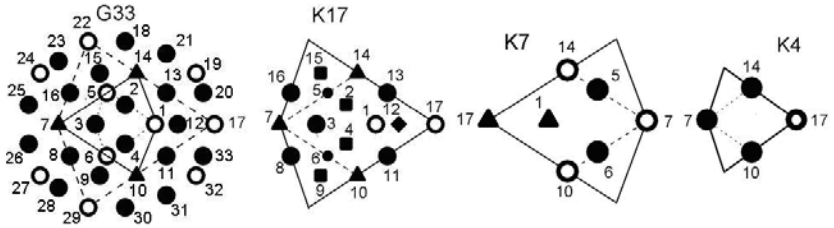

Fig. 1. Types of clusters. Different types of atoms are marked with various shapes.

For instance: $Al_{71}TM_{29}$ versus (34:38):28 in the K7. Kite-clusters can be then used as a very good initial model for the further refinement. Some geometrical, as well as statistical and analytical features of kite-clusters have been described in [1] and [2]. This paper is focused on the relations between kite-clusters. Some techniques for transforming one into another are provided. The cluster model is also compared to the rhombus model. It is pointed out when these two models are fully equivalent. Knowledge of such cases makes the refinement process more efficient, as the rhombus model is more flexible and much easier to deal with when it comes to analytical and statistical calculations.

[1] J. Wolny, B. Kozakowski, Phil. Mag. **86** (2006) 637.
[2] A. Dabrowska, B. Kozakowski, J. Wolny, Acta Cryst. **A61** (2005) 350.

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