MS27-O3

Application of the Generalized Penrose Tiling to the structure refinement of AlCuRh decagonal quasicrystal

Radosław Strzałka[1], Ireneusz Bugański[1], Maciej Chodyń[1], Janusz Wolny[1]

1. Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland

email: strzalka@fis.agh.edu.pl

In our presentation we will show the refinement results of the AlCuRh decagonal quasicrystals with application of the Generalized Penrose tiling (GPT) as a quasilattice. The applicability of the GPT to structural modeling of decagonal systems was widely studied by Chodyn et al. [1], whereas the atomic structure of AlCuRh was previously investigated by Kuczera et al. [2]. In both papers [1,2], as well as in our studies, the statistical method based on the average unit cell concept was used [3]. The GPT-based model consists of additional fifth atomic surface, which size is dependent on the shift along z-axis in multidimensional hyperspace. Alongside, all other pentagonal atomic surfaces become non-uniform decagons. The subdivision of the atomic surfaces (as well as average unit cells) into regions corresponding to a particular structural unit (thick of thin rhombus) at a given orientation gives now hexagons instead of triangles. All these features of the GPT introduce completely new local arrangements of thick and thin rhombi, not observed for the regular Penrose tiling. A quasilattice obtained from the GPT gives more freedom in the refinement, which is promising in achieving better refinement results of real systems. The GPT model was already applied to model decagonal quasicrystals and simple decorations with atoms. Now we show the refinement results for the decagonal AlCuRh. This is the first application of the GPT to real decagonal system in literature. The starting decoration was derived from the electron density maps, obtained from the diffraction data collected previously by Kuczera. New families of unit tiles' arrangement (created by the additional fifth atomic surface) were decorated in the same manner as all others. The refinement was converged with R-factor of 6.52%, which is a significant improvement comparing to 7.9% reported in the original paper [2]. The comparison of the two models will be presented and details of the new results will be discussed.

References:

[1] Chodyn, M., Kuczera, P., Wolny, J. (2015). Acta Cryst. A, 71, 161-168.
[2] Kuczera, P., Wolny, J., Steurer, W. (2012). Acta Cryst. B, 68, 578-589.

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Is PdBi the little brother of AuIn?

Laura Folkers[1], Sven Lidin[1]

1. Department of Chemistry, Lund University, Lund, Sweden

email: laura.folkers@chem.lu.se

Recently the structure of the AuIn 1:1 phase was elucidated [1], showing its structural changes with temperature. The first indicators for uncommon behaviour in AuIn was the fact that the structure was unknown, despite the simple stoichiometry. A second peculiarity is the difficulty of growing a single crystal of this material. However the main indicator is the Differential Scanning Calorimetry (DSC) data shown in the top panel of Figure 1. At a temperature of 443°C the DSC curve signals the melt of a super structure, while the full structure only melts at 515°C. Only with this information growth of a suitable single crystal was possible, and this could be used to obtain the here presented diffraction data. This data showed that AuIn, believed to be of the thallium iodide type [2], actually only shows this structure above the temperature of 443°C and at lower temperatures undergoes first a Peierls type distortion before it becomes incommensurate [1].

PdBi turns out to be a similar case, where a 1:1 intermetallic, which normally display simple structures turns out to be quite complex. The atomic positions of the reported structure of the HT phase of this compound correspond to the TlI type structure [3].

Even more importantly, the DSC measurement shows precisely the same pattern as for AuIn (see Fig.1, bottom). A first melting event occurs at 583°C, a second one at 635°C and a solidification peak can be seen at 569°C.

A recent synchrotron study of PdBi shows that it indeed follows the expected behaviour. Between room temperature and 300°C, preliminary data treatment has shown that the structure transforms from a commensurate 2x2x2 super structure, via an incommensurate structure, to a disordered structure. This is indicated by satellite positons slightly changing place and eventually satellites turning into diffuse scattering.

The precise behaviour of PdBi with respect to temperature will be discussed in detail in the presentation.