

MS27-O3**Application of the Generalized Penrose Tiling to the structure refinement of AlCuRh decagonal quasicrystal**Radosław Strzalka¹, Ireneusz Bugański¹, Maciej Chodyń¹, Janusz Wolny¹¹. 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.**Keywords:** decagonal AlCuRh, generalized Penrose tiling, statistical method**MS27-O4****Is PdBi the little brother of AuIn?**Laura Folkers¹, Sven Lidin¹¹. 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].

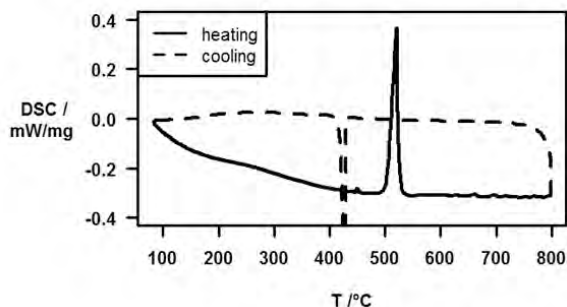
PdBi turns out to be a similar case, where a 1:1 intermetallic, which normally display simple structures turns out to be quite complex. The atomic positions of the reported structure of the HT phase of this compound correspond to the TII type structure [3].

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.

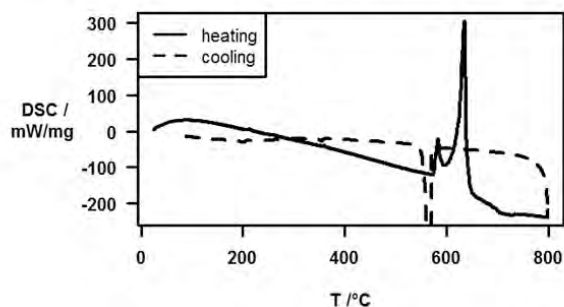
A recent synchrotron study of PdBi shows that it indeed follows the expected behaviour. Between room temperature and 300°C, preliminary data treatment has shown that the structure transforms from a commensurate 2x2x2 super structure, via an incommensurate structure, to a disordered structure. This is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

DSC measurement of AuIn sample



DSC measurement of PdBi sample



References:

- [1] Folkers, L. C. & Simonov, A. & Wang, F. & Lidin, S. (2018), *Inorg. Chem.*, 57, 2791 - 2796.
 [2] Schubert, K. & Rösler, U. & Kluge, M. & Anderko, K. & Härle, L. (1953), *Naturwissenschaften*, 40, 34.
 [3] Zhuravlev, N. N. (1957), *Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki*, 5, 1064 - 1072.

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MS27-05

Adventures in modulation: derivatives of barluenga's reagent

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Single-crystal X-ray diffraction is a powerful technique: as the technique has developed data collections have been getting faster and faster, and structure determination is becoming more routine. There are an increasing number of non-expert users collecting data, solving and refining structures before publishing their own results. However, with the advent of higher intensity laboratory X-ray sources, easier access to synchrotron radiation and more sensitive detectors, more and more molecular structures are showing alien features beyond the realms of conventional crystallography [1].

Though the concept of modulated structures is now fairly well established in solid state chemistry, the abundance of reported modulated molecular materials is less than might be expected. There are a number of probable reasons for this, including the fact that the synthetic chemist is primarily interested in connectivity and proof of what they have made, so they are not curious about additional peaks seen in a diffraction pattern. When tweaking the synthesis and/or changing crystallisation conditions makes the curious extra features disappear, this is typically the chosen route and the original structure is casually swept under the carpet.

When a concerted effort is made to study the appearance of additional satellite reflection and relating it to changes within the structure, valuable extra information can be gained concerning molecular packing and the crystalline state. One such example is found in Barluenga's reagent, IPy_2BF_4 (Py = pyridine) [2], which has been shown to exhibit a transient modulated phase on cooling (see image). Systematic studies on derivatives of Barluenga's reagent have been carried out in which the pyridine is replaced with 2,4,6-trimethyl pyridine (collidine, Coll), iodine with bromine and the BF_4 anion is replaced with other small anions including ClO_4 and PF_6 [3]. Through these changes to the chemistry we can begin to understand how the crystal structure and the diffraction pattern are related and why satellite peaks may appear, with the aim of improving our understanding of the mechanism governing the appearance of modulation in molecular materials.