Is PdBi the little brother of AuIn?

Laura C. Folkers, Sven Lidin

Lund University, Naturvetarvägen 14, 223 62 Lund, Sweden

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 Figure 1.

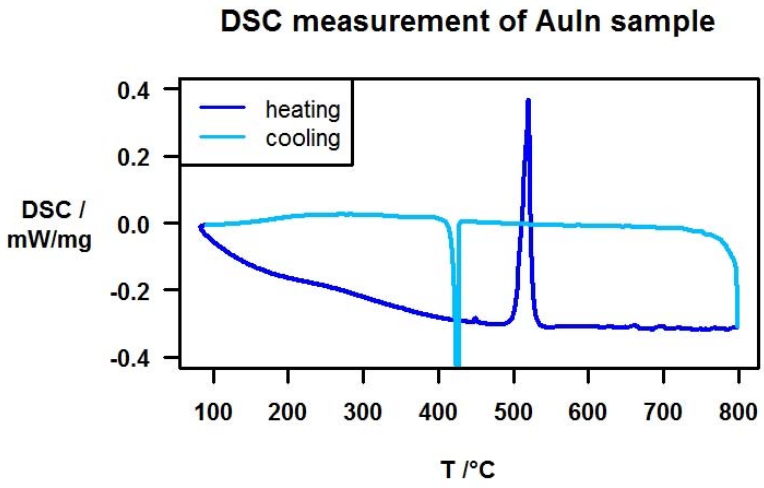

Figure 1: Differential Scanning Calorimetry plot of AuIn 1:1 mixture. The dark blue line shows the heating curve and the light blue line shows the cooling curve. At a temperature of 443 °C a first melting event occurs in the heating curve and the full structure melts at 515°C. Hence the first melting event is attributed to a superstructural melt.

At a temperature of 443°C the DSC curve signals the melt of a super structure, which cannot be ignored on crystal growth. Hence this information made growth of a suitable single crystal possible, from which diffraction data was obtained. 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.2).

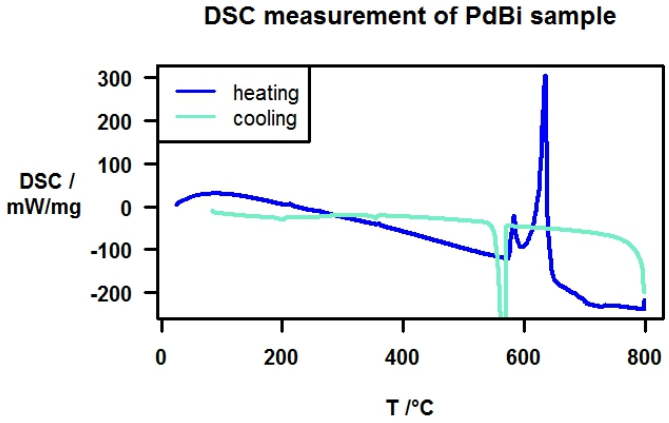

Figure 2: DSC measurement of PdBi, the solid black curve denotes the heating curve and the broken off curve denotes the cooling curve. A first melting event occurs at 583°C, a second one at 635°C and a solidification peak can be seen at 569°C. Also here the first melting peak is attributed to a superstructural melt.

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 (Fig. 3).

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

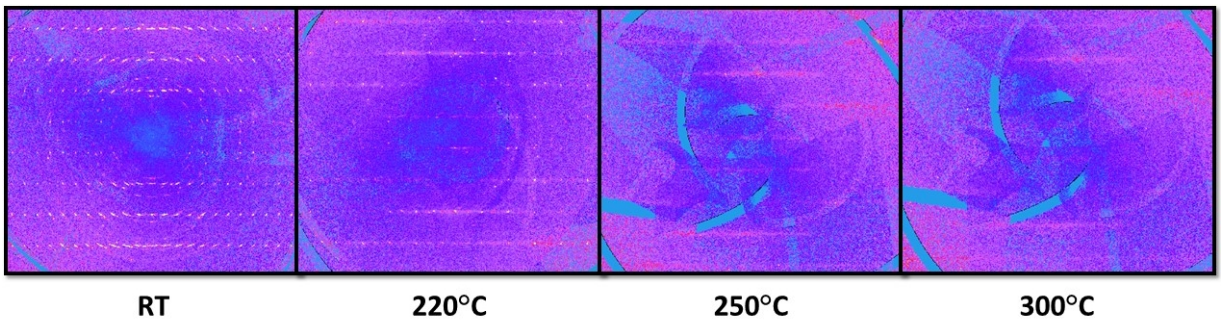

Figure 3: Reciprocal space images of PdBi. The room temperature layer is 1kl, all others are 1.5kl. This figure shows how PdBi changes from a commensurate super structure at room temperature to an incommensurate structure at 220°C and after that becomes gradually more disordered.

1. L. C. Folkers, A. Simonov, F. Wang, S. Lidin, *Inorg. Chem.*, **57**, (2018), 2791.

2. K. Schubert, U. Rösler, M. Kluge, K. Anderko, L. Härle, *Naturwissenschaften*, **40**, (1953), 34

3. N. N. Zhuravlev, *Zhurnal Eksperimental'noi i Teoreticheskoi Fiziki'*, **5**, (1957), 1064.

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