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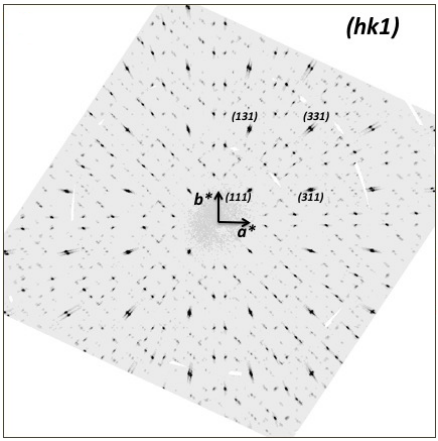

Figure 1. (hk1) reciprocal plane of $Pr_2NiO_{4.25}$ containing incommensurate superstructure reflections along ^{2} with main reflections @RT reconstructed from X-ray single crystal diffraction data obtained on a STOE STADIVARI *diffractometer (Mo Ka µ-focus) equipped with a 2D Pilatus detector .*

Keywords: Hole doped, Incommensurate modulation, Oxygen/charge ordering

MS26-P2 The mystery of the AuIn 1:1 phase

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Recently, the Gold Indium system has regained interest due to its importance for applications in soldering and nanowire growth. For these applications knowledge of the occurring components in the phase diagram is important. Earlier studies of this alloy were able to uncover most currently known compounds along with their crystal structures. Only the structure of the seemingly most straight-forward one, AuIn 1:1, has not been elucidated. Its lattice parameters are known from earlier experiments [1], but growth of single crystals has proved difficult.

The powder diffraction pattern contains unindexed peaks that cannot be explained by any known Au-In binary or by any known oxide or nitride. The problem is exacerbated by the tendency of the compound to amorphisize on grinding. Subsequent annealing at low temperature (400°C) however restores full crystallinity.

Differential thermal analysis (DTA conf. Fig. 1) reveals further surprises. On heating, a small endothermic peak appears at 440°C while a second endotherm at 515°C corresponds well with the reported melting point of AuIn (T_M = 510°C [2]). On cooling only one exothermic peak can be observed, which, in position, corresponds to the low temperature exotherm at 440°C, but in size it corresponds to the high temperature endotherm at 515°C.

An electron diffraction study reveals weak satellites in AuIn, indicating that the structure may be incommensurately modulated [3].

In this study we will discuss structure models for AuIn and possible explanations for the thermal behaviour.

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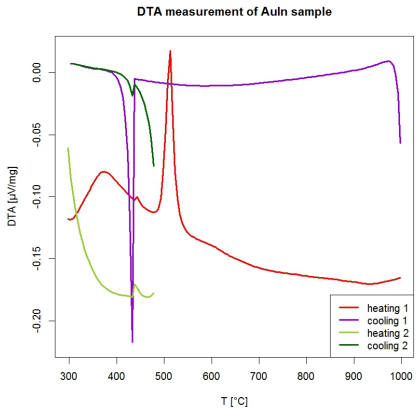

Figure 1. DTA curve showing a first melt at T = 440°C, a second one at T = 515°C and solidification at T = 436°C.

Keywords: Intermetallics, modulation, powder diffraction

MS26-P3 $ErCu_{0.5}Ga_{3.5}$ – A (3+1)D-incommensurately modulated variant of the $BaAl_4$ type

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Ternary intermetallic systems R-Cu-Ga were widely studied for all the rare earth metals and uranium [1,2]. The gallium rich intermediate phases RCu_xGa_{4-x} were reported to crystallize as tetragonal or orthorhombically distorted derivatives of the $BaAl_4$-type structure [3]. Moreover, some of these phases tend to form modulated structures due to disorder that might occur in the R and/or Cu/Ge crystal sublattices [4].

Single crystals of the ternary compound $ErCu_{0.5}Ga_{3.5}$ were grown by the self-flux method. The structure of $ErCu_{0.5}Ga_{3.5}$ was determined by single-crystal X-ray diffraction recorded at 120 and 300 K. The compound crystallizes in an incommensurately modulated (3+1)D structure, being related to the tetragonal $BaAl_4$ -type. The structure was refined in the monoclinic superspace group $X2/m(\alpha,0,g)00$, with modulation vector q = (0.184(2), 0, 0.347(1)), a = 413.99(9), b = 963.83(11), c = 410.52(16) pm, and b = 90.11(1)° at 120 K. The modulation wave occurs in the Ga/Cu disordered sublattice and q was found to be similar at both temperatures. Furthermore, analysis of the reciprocal pattern of $ErCu_{0.5}Ga_{3.5}$ also indicates a twinning effect, described by a two-fold axis around a^*.

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Keywords: incommensurate, occupation modulation, intermetallics