



Figure 1. DTA curve showing a first melt at $T = 440^{\circ}\text{C}$, a second one at $T = 515^{\circ}\text{C}$ and solidification at $T = 436^{\circ}\text{C}$.

Keywords: Intermetallics, modulation, powder diffraction

MS26-P3 $\text{ErCu}_{0.5}\text{Ga}_{3.5} - \text{A}$
(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 $\text{RCu}_x\text{Ga}_{4-x}$ 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 $\text{ErCu}_{0.5}\text{Ga}_{3.5}$ were grown by the self-flux method. The structure of $\text{ErCu}_{0.5}\text{Ga}_{3.5}$ 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 $b = 90.11(1)^\circ$ 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 $\text{ErCu}_{0.5}\text{Ga}_{3.5}$ also indicates a twinning effect, described by a two-fold axis around a^* .

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