ABSTRACT CODE

X-ray investigation of $Th_3M_2M'_3$ alloys

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In recent years we focused our attention on a study of the crystal and magnetic structure of $U_3M_2M'_3$ compounds with M = Al, Ga and M'= Si, Ge [1 – 4], which all were found to crystallize in a new structure type ($U_3Ga_2Ge_3$), with space group *I*4, a low-symmetry derivative of the Cr_5B_3 anti-type structure (space group *I4/mcm*). Neutron diffraction on a single crystal $U_3Al_2Si_3$ revealed a non-collinear ferromagnetic spin structure for the uranium atoms in the eight-fold position [4]. For proper derivation of the uranium ground-state from low temperature specific heat measurements on these materials, however, comparison with an isotypic nonmagnetic material would be of benefit. We decided to inspect the homologous systems Th-M-M' and in our paper we present analysis of our X-ray powder diffraction measurements.

Alloys $Th_3M_2M'_3$ were prepared by arc-melting starting from a nominal composition, 37.5 at.% Th, 25.0 at.% Al or Ga and 37.5 at.% Si or Ge. Final chemical composition was checked by EMPA. Precise lattice parameters and standard deviations were obtained from a least squares refinement of room temperature Guinier-Huber image plate X-ray powder data, using monochromatic $CuK_{\alpha 1}$ radiation with an internal standard of 6N-pure Ge (a_{Ge} = 0.5657906 nm at RT). The Rietveld refinements were performed using the GSAS software package.

No ternary compounds were observed bearing isotypism with the homologous $U_3Ga_2Ge_3$ type of structure. The majority phase for all compounds is the tetragonal $\alpha ThSi_2$ type $Th(M_{1-x}M'_x)_2$ (space group $I4_1/amd$). The secondary phase in Si-alloys is an orthorhombic phase of the FeB type (Pnma). While $Th_3Al_2Si_3$ consists only from these two phases [$Th(Al_{1-x}Si_x)_2$ and $Th(Al_{1-x}Si_x)$], the phase composition of $Th_3Ga_2Si_3$ was found to be more complicated. The second phase in Ge-alloys was identified as face centered cubic of the NaCl type $Th(Al_{1-x}Ge_x)$ and/or $Th(Ga_{1-x}Ge_x)$ (space group $Fm\bar{3}m$).

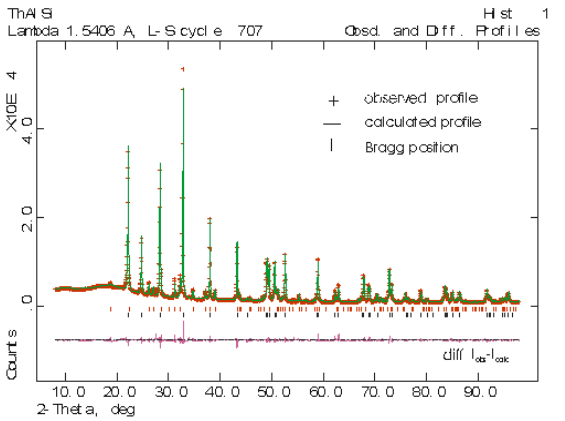

Fig. 1. X-ray data taken from $Th_3Al_2Si_3$ alloy, calculated profile and Bragg positions.

References

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