Poster

Crystal structures of the phases in the systems T_5M_3–$T_5M'_3$ (T = Ti, Zr, Hf; M = Al, Ga; M' = Si, Ge, Sn, Pb, Sb, Bi)

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In the ternary systems T–M–M' (T = Ti, Zr, Hf; M = Al, Ga; M' = Si, Ge, Sn, Pb, Sb, Bi) in the cross-section T_5M_3–$T_5M'_3$ at 600°C phases with four structure types are observed: Mn_5Si_3 – **A** (Pearson symbol *hP*16, space group $P6_3/mcm$), W_5Si_3 or its ternary ordered variant Nb_5SiSn_2 – **B** (*tI*32, $I4/mcm$), Yb_5Sb_3 – **C** (*oP*32, *Pnma*), and Y_5Bi_3 – **D** (*oP*32, *Pnma*). The closely related structure type Hf_5CuSn_3 – **E** (*hP*18, $P6_3/mcm$), which is a filled ternary variant of the structure type Mn_5Si_3 and a ternary ordered variant of the structure type Ti_5Ga_4, exists in some of these systems at a neighboring composition [1].

Table. Structure types of phases in the systems T_5M_3–$T_5M'_3$ (T = Ti, Zr, Hf; M = Al, Ga; M' = Si, Ge, Sn, Pb, Sb, Bi) at 600°C (data at other temperatures are given in italics; solid solutions based on binary phases are indicated by parentheses; × no binary compound; * no data available).

	System					
	Ti_5M_3–$Ti_5M'_3$		Zr_5M_3–$Zr_5M'_3$		Hf_5M_3–$Hf_5M'_3$	
M'	M = Al	M = Ga	M = Al	M = Ga	M = Al	M = Ga
Si	× – (***A***)	**B** – (***A***)	× – **B** – **(A)**	**(*A*) – (*A*)**	× – **A** – **(A)**	**(A)**
Ge	× – (***A***)	**B** – (***A***)	× – **B** – **E** – **(A)**	**A – A**	× – **A** – **E** – **(A)**	**(A)**
Sn	× – ***B*** – (***A***)	**(*B*) – *B* – A**	× – **B** – **B** – **(A)**	**(A) – B – (A)**	× – **A** – **B** – **(E)**	**(A) – B – (E)**
Pb	× – ***B*** – ×	**B** – ×	× – ***B*** – **(A)**	**A – A**	× – ***B*** – ×	**A** – ×
Sb	× – ***B*** – **C**	**B – (*A*) – B – C**	× – **B** – **B** – **(A)**	**(A) – B – (A)**	× – **A** – **B** – **E** – **(D)**	**(A) – B – E – (D)**
Bi	*	**B** – ×	× – **A**	**A – A**	*	**A** – ×

Continuous solid solutions with Mn_5Si_3-type structure form in the systems Hf–Ga–{Si,Ge} at 600°C. Limited solid solutions $T_5M_{3-x}M'_x$ of substitution type with the same structure type exist in the systems Ti–Ga–Sb (at 400°C), Zr–Ga–Si (at 800°C), and Hf–{Al,Ga}–{Sn,Sb} (at 600°C), and limited solid solutions $T_5M_xM'_{3-x}$ in the systems Ti–Al–Si (at 700°C), Ti–Al–Ge (1000°C), Ti–Al–Sn (at 900°C), Ti–Ga–{Si,Ge} (at 800°C), Zr–Al–{Si,Ge,Sn} (at 600°C), Zr–Ga–Si (at 800°C), Zr–Ga–{Sn,Sb} (at 600°C), Hf–Al–{Si,Ge} (at 600°C), and Hf–{Al,Ga}–{Sn,Sb} (at 600°C). A limited solid solution $Ti_5Ga_{3-x}Sn_x$ of substitution type with W_5Si_3-type structure has been reported in the system Ti–Ga–Sn (at 1300°C), individual ternary compounds $T_5(M_{1-x}M'_x)_3$ with W_5Si_3/Nb_5SiSn_2-type structure exist in the systems Ti–Al–Sn (at 900°C), Ti–{Al,Ga}–Sb (at 400°C), {Zr,Hf}–{Al,Ga}–{Sn,Sb} (at 600°C), and {Ti,Zr,Hf}–Al–Pb (at 900°C), whereas limited solid solutions $Hf_5M_xSb_{3-x}$ with Y_5Bi_3-type structure were revealed in the systems Hf–{Al,Ga}–Sb (at 600°C).

In the systems Hf–{Al,Ga}–Sb (at 600°C) the formation of the solid solutions $Hf_5M_xSb_3$ of inclusion type with Hf_5CuSn_3-type structure was observed. The structure type Hf_5CuSn_3 was also found for individual ternary compounds $T_5MM'_3$ in the systems {Zr,Hf}–Al–Ge (at 600°C) and Hf–{Al,Ga}–Sb (at 600°C).

[1] Pearson's Crystal Data, Crystal Structure Database for Inorganic Compounds, Release 2023/24, Eds. P. Villars, K. Cenzual, ASM International, Materials Park, Ohio, USA.