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Single-crystal investigation of the $EuCu_8Ga_5$ and $YbCu_5Ga_7$ phases

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Two new ternary phases, $EuCu_8Ga_5$ and $YbCu_5Ga_7$, were prepared by arc-melting. Their crystal structures were investigated on single-crystal X-ray diffraction data. The above mentioned phases crystallize with known structure types, namely, $NaZn_{13}$ and $ThMn_{12}$, respectively. Details of the structures (interatomic distances, coordination of the atoms) are briefly discussed.

Intermetallics / Crystal structure / X-ray diffraction

Introduction

Ternary rare earth – copper – gallium systems and compounds have been widely studied during the past decades. The phase diagrams have been studied in the whole concentration region, or in part of it, for all the rare-earth metals: Sc–Cu–Ga [1], Y–Cu–Ga [2,3], {La, Ce, Pr, Nd}–Cu–Ga [4], Sm–Cu–Ga [5], {Eu, Yb}–Cu–Ga [6], {Gd, Tb}–Cu–Ga [7], Dy–Cu–Ga [8], Ho–Cu–Ga [9], {Er, Tm}–Cu–Ga [10], and Lu–Cu–Ga [11]. Crystal structures of ternary *R*–Cu–Ga compounds have also been reported in [12] and [13]. Summarized data on the interaction between rare-earth, copper and gallium metals is given in Table 1.

The Eu–Cu–Ga and Yb–Cu–Ga ternary systems have been investigated at 500°C for $R \leq 33.3$ at.%. Three ternary compounds, $EuCu_{9.5-6.7}Ga_{3.5-6.3}$ ($NaZn_{13}$-type), $EuCu_{1.1-0.2}Ga_{2.9-3.8}$ ($BaAl_4$-type), and $EuCu_{0.14}Ga_{2.86}$ ($CeNiSi_2$-type), were identified in the Eu–Cu–Ga system. The Yb–Cu–Ga system is characterized by the existence of ten ternary phases: $YbCu_{7.4}Ga_{5.6}$ ($NaZn_{13}$-type), $YbCu_{6.4-5.0}Ga_{5.6-7.0}$ ($ThMn_{12}$-type), $Yb_2Cu_{12.8-8.5}Ga_{4.2-8.5}$ (Th_2Zn_{17}-type), $YbCu_{3.6}Ga_{2.4}$ (YCd_6-type), $YbCu_{4.7}Ga_{0.3}$ ($AuBe_5$-type), $YbCu_{3.8-2.9}Ga_{1.2-2.1}$ ($CaCu_5$-type), $YbCu_{1.25-0.25}Ga_{2.75-3.75}$ ($BaAl_4$-type), $YbCu_{0.15}Ga_{3.85}$ ($CaCu_{0.15}Ga_{3.85}$-type), $Yb_3Cu_{4.4-3.3}Ga_{6.6-7.7}$ (La_3Al_{11}-type), and $YbCu_{0.08}Ga_{2.92}$ ($CeNiSi_2$-type).

The present work is part of a systematic investigation of ternary gallium-based alloy systems containing europium and ytterbium. Herein, we show results on the crystal structures of the $EuCu_8Ga_5$ ($NaZn_{13}$-type) and $YbCu_5Ga_7$ ($ThMn_{12}$-type) phases, investigated by single-crystal X-ray diffraction.

Experimental details

The samples were prepared using europium, ytterbium, copper and gallium with nominal purity better than 99.95 wt.%. Small, surface-cleaned pieces were put inside a carbon glass crucible, sealed inside quartz tubes under vacuum, and reacted at 900°C. The obtained metallic-like products were further annealed at 400°C for 20 days. X-ray phase analysis of the alloys was carried out using a PANalytical X'Pert Pro diffractometer with Cu *K*α-radiation.

Single crystals suitable for X-ray data collection were extracted from crushed single phase samples. A four-circle Enraf Nonius Mach III diffractometer with graphite monochromated Mo *K*α-radiation and a scintillation counter with pulse height discrimination were used for collecting the data. Scans were taken in the $\omega/2\theta$ mode. Empirical absorption corrections were applied on the basis of Ψ-scan data. The crystal structures were refined using SHELXL-97 [14] (full-matrix least-squares on F^2). The unit cell parameters were obtained by least-squares refinement of the 2θ values of 25 intense and well-centered reflections from various parts of the reciprocal space ($15° < 2\theta < 35°$).

Results and discussion

The $EuCu_8Ga_5$ phase

The investigation of the $EuCu_8Ga_5$ crystal structure was made on a cubic-shape single crystal extracted from an annealed $Eu_7Cu_{57}Ga_{36}$ alloy. Details on the data collection and the structure refinements

Table 1 Summarized data on phase diagrams and ternary phases with established structure for the *R*–Cu–Ga (*R* = Sc, Y, La–Lu) systems.

R / Phase	at.%	Sc	Y	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
$R(Cu;Ga)_{13}$	7.1	–	–	A B	A B	A B	A	–	A	A	–	–	–	–	–	–	A	–
$R(Cu;Ga)_{12}$	7.7	C	C	–	–	–	–	–	C	–	C	C	C	C	C	C	C	C
$R(Cu;Ga)_{11}$	8.3	–	D	–	D	D	D E	–	D E F	–	D F	D	D	–	–	–	–	–
$R_2(Cu;Ga)_{17}$	10.5	–	G	–	–	–	G	–	G	–	G	G	G	G	G	G	G	G
$R(Cu;Ga)_6$	14.3	H I	–	–	–	–	–	–	–	–	–	–	–	–	–	–	I	I
$R(Cu;Ga)_5$	16.7	–	–	–	–	–	–	–	–	–	–	J	J	J	J	J	J K	J L
$R_{13}(Cu;Ga)_{58}$	18.3	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–	M
$R(Cu;Ga)_4$	20	–	N	N	N	N	N	–	N	N	N	N	N	–	–	–	N O	–
$R_3(Cu;Ga)_{11}$	21.4	–	P	–	–	–	–	–	–	–	–	–	P	P	P	P	P	P
$R_{14}(Cu;Ga)_{51}$	21.5	R	R	–	–	–	R	–	R	–	R	R	R	R	R	R	–	R
$R(Cu;Ga)_3$	25	S	T	–	–	–	–	–	–	U	–	–	–	–	–	–	U	–
$R(Cu;Ga)_2$	33.3	V W	W	V	X	X	X	–	X	–	V X	V X	V X	V X	V X	V X	–	V X
System	–	▲	▲	Δ	Δ	Δ	Δ	–	Δ	Δ	Δ	Δ	Δ	▲	Δ	Δ	Δ	Δ

Structure types: A – $NaZn_{13}$, B – $CeNi_{8.5}Si_{4.5}$, C – $ThMn_{12}$, D – $BaCd_{11}$, E – $SmZn_{11}$, F – $SmCu_{6.2}Ga_{4.8}$, G – Th_2Zn_{17}, H – $HfNi_2Ga_4$, I – YCd_6, J – $CaCu_5$, K – $AuBe_5$, L – $EuMg_5$, M – $Gd_{13}Zn_{58}$, N – $BaAl_4$, O – $CaCu_{0.15}Ga_{3.85}$, P – La_3Al_{11}, R – $Gd_{14}Ag_{51}$, S – $MnCu_2Al$, T – $MgCuAl_2$, U – $CeNiSi_2$, V – $CeCu_2$, W – $CaIn_2$, X – AlB_2. Phase equilibrium has been investigated in the whole concentration range (0-100 at.% *R*) (▲) or in part of it (0-33.3 at.% *R*) (Δ).

are given in Table 2. The atom coordinates and the thermal anisotropic parameters are shown in Tables 3 and 4, respectively. The present experiment fully confirms the structural model previously reported in [6], *i.e.* the $NaZn_{13}$ type. Although the Cu and Ga atoms are not easily distinguishable by X-ray diffraction, our refined model seems to be most stabilized when the Cu atoms are located in the 8*b* site. The occupancy parameters of the atoms were refined in a separate series of least-squares cycles checking the correctness of the composition. Full occupation was observed for all the atom sites and the composition of the phase was assumed to be $EuCu_8Ga_5$. It should be noted that the results presented here are similar to those reported in [15], where studies were performed on the slightly deficient composition $EuCu_{6.5-x}Ga_{6.5}$ ($x \sim 0.2$).

The unit cell and the coordination polyhedra for the atoms in $EuCu_8Ga_5$ can be seen in Fig. 1*a*. In this $NaZn_{13}$-type phase, the Eu atoms occupy the positions of the Na atoms, while the Cu and *M* (0.58Cu and 0.42Ga) atoms occupy the two sites of the Zn atoms. The interatomic distances and the coordination numbers are presented in Table 5. The Eu atoms are coordinated by 24 neighboring *M* atoms (at a distance of 3.450(1) Å), which form distorted pseudo Frank-Kasper polyhedra. The icosahedral environment of the Cu atoms is also composed by *M* atoms (12 × 2.563(1) Å). Ten *M*, one Cu and two Eu atoms form the coordination sphere (pseudo Frank-Kasper polyhedron) of the *M* atoms. The shortest *M*–*M* distances range from 2.478(1) to 2.877(2) Å.

$NaZn_{13}$-type phases are already known in many binary and ternary systems [13]. This structure can be seen as a packing of large sodium atoms and groups composed by small zinc atoms (isolated icosahedra $[ZnZn_{12}]$) in a CsCl-type like manner (Fig. 2). To our best knowledge, five ternary structures with the composition $A(B;C)_{13}$ are known, where similar ordering of the atoms is observed (Fig. 2). They can be described as deformed variants of the cubic $NaZn_{13}$ type (with lattice parameter a_0) [16]: the tetragonal $CeNi_{8.5}Si_{4.5}$ type (space group *I*4/*mcm*, $a \sim a_0/\sqrt{2}$, $c \sim a_0$) [16], tetragonal $SrNi_{6.3}Si_{6.7}$ type (space group *P*4/*nbm*, $a \sim a_0/\sqrt{2}$, $c \sim a_0$) [17], orthorhombic $LaNi_{7.36}In_{5.64}$ type (space group *Ibam*, $a \sim a_0/\sqrt{2}$, $b \sim a_0/\sqrt{2}$, $c \sim a_0$) [18], orthorhombic $SrCu_7In_6$ type (space group *Pnnm*, $a \sim a_0$, $b \sim a_0$, $c \sim a_0$) [19], and the orthorhombic $SrNi_{7.9}In_{5.1}$ type (space group *Cccm*, $a \sim a_0\sqrt{2}$, $b \sim a_0\sqrt{2}$, $c \sim a_0$) [20].

The $YbCu_5Ga_7$ phase

Irregular light silvery crystals were isolated from the crushed $Yb_{7.7}Cu_{38.5}Ga_{53.8}$ alloy and their quality was tested. Crystal structure investigations were performed in similar manner as for the previous compound ($EuCu_8Ga_5$). Experimental details of the crystal structure refinement of $YbCu_5Ga_7$ are given in Tables 2, 6 and 7. The crystal structure of this phase adopts the $ThMn_{12}$ type. The Yb atoms occupy the 2*a* site. Due to the similar scattering power of copper and gallium atoms, additional considerations (interatomic distances and preferential occupation of atoms in

Table 2 Crystallographic data and structure refinements of the $EuCu_8Ga_5$ and $YbCu_5Ga_7$ phases.

Phase	$EuCu_8Ga_5$	$YbCu_5Ga_7$
Structure type	$NaZn_{13}$	$ThMn_{12}$
Crystal system	Cubic	Tetragonal
Space group	*Fm*-3*c*	*I*4/*mmm*
Person symbol	*cF*112	*tI*26
Lattice parameters:		
a	11.8850(15) Å	8.6135(5) Å
c	–	5.1214(8) Å
V	1678.8(4) Å^3	379.97(7) Å^3
Molar mass	1008.88 g/mol	978.78 g/mol
Formula units per cell	8	2
Calculated density	7.983 g/cm^3	8.555 g/cm^3
Crystal shape and color	Cubic, Silvery	Irregular, Silvery
Diffractometer	Enraf-Nonius Mach III	Enraf-Nonius Mach III
Wavelength	Mo-*K*α (λ = 0.71073 Å)	Mo-*K*α (λ = 0.71073 Å)
Monochromator	Graphite	Graphite
Temperature	293(2) K	293(2) K
Absorption coefficient	42.812 mm^{-1}	50.109 mm^{-1}
F(000)	3600	864
θ range for data collection	3.43º to 39.68º	3.34º to 44.80º
Scan type	ω-2θ	ω-2θ
Range in *hkl*	±16, ±10, ±10	±14, ±14, ±8
Total no. reflections	2723	4961
Independent reflections	147	424
Reflections with $I > 2\sigma(I)$	126	368
R_σ, R_{eq}	0.0689, 0.1416	0.0527, 0.1649
Structure refinement	SHELXL-97	SHELXL-97
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	147/0/10	424/0/16
Goodness-of-fit on F^2	1.040	1.069
Final *R* indices [a]	*R*1 = 0.0433, *wR*2 = 0.0803	*R*1 = 0.0307, *wR*2 = 0.0532
R indices (all data)	*R*1 = 0.0510, *wR*2 = 0.0839	*R*1 = 0.0389, *wR*2 = 0.0551
Weighting scheme [b]	*a* = 0.0465, *b* = 0	*a* = 0, *b* = 0
Extinction coefficient	0.00057(10)	0.0029(2)
Largest diff. peak/hole	2.783/-2.167 e/Å^3	3.303/-2.423 e/Å^3

[a] $R1 = \sum(||F_o|-|F_c||)/\sum|F_o|$, $wR2 = \{\sum w[(F_o^2-F_c^2)^2]/\sum w[(F_o^2)^2]\}^{½}$;
[b] $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, where $P = (F_o^2+2F_c^2)/3]$.

Table 3 Atom coordinates and isotropic displacement parameters for $EuCu_8Ga_5$.

Atom	Site	*x*	*y*	*z*	U_{eq} (Å^2)
Eu	8*a*	¼	¼	¼	0.0045(4)
Cu	8*b*	0	0	0	0.0082(7)
M	96*i*	0	0.12102(9)	0.17853(8)	0.0068(4)

M = 0.58Cu + 0.42Ga

Table 4 Anisotropic displacement parameters for $EuCu_8Ga_5$ (Å^2).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Eu	0.0045(4)	0.0045(4)	0.0045(4)	0	0	0
Cu	0.0082(7)	0.0082(7)	0.0082(7)	0	0	0
M	0.0060(6)	0.0091(6)	0.0051(7)	0.0024(3)	0	0

Table 5 Interatomic distances (*d*) and coordination numbers (CN) of the atoms in the structures of $EuCu_8Ga_5$ and $YbCu_5Ga_7$.

Atoms	*d* (Å) / CN	Atoms	*d* (Å) / CN	Atoms	*d* (Å) / CN
$EuCu_8Ga_5$		$YbCu_5Ga_7$			
Eu–	24	Yb–	20	Ga–	14
–24*M*	3.450(1)	–4Ga	2.986(1)	–4Cu	2.640(1)
		–8*M*	3.152(1)	–1Ga	2.642(1)
Cu–	12	–8Cu	3.304(1)	–2*M*	2.799(1)
–12*M*	2.563(1)			–2*M*	2.806(1)
		Cu–	12	–1Yb	2.986(1)
M–	13	–4*M*	2.525(1)	–4Ga	3.170(1)
–2*M*	2.478(1)	–2Cu	2.561(1)		
–1Cu	2.563(1)	–4Ga	2.640(1)	*M*–	12
–2*M*	2.650(1)	–2Yb	3.304(1)	–4Cu	2.525(1)
–4*M*	2.653(1)			–2*M*	2.600(1)
–1*M*	2.877(2)			–2Ga	2.799(1)
–2Eu	3.450(1)			–2Ga	2.806(1)
–1*M*	3.505(2)			–2Yb	3.152(1)

Table 6 Atom coordinates and isotropic displacement parameters for $YbCu_5Ga_7$.

Atom	Site	*x*	*y*	*z*	U_{eq} (Å^2)
Yb	2*a*	0	0	0	0.00343(10)
Cu	8*f*	¼	¼	¼	0.00633(14)
Ga	8*i*	0.34662(8)	0	0	0.00753(14)
M	8*j*	0.28654(12)	½	0	0.01338(19)

M = 0.25Cu + 0.75Ga

Table 7 Anisotropic displacement parameters for $YbCu_5Ga_7$ (Å^2).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Yb	0.00208(12)	0.00208(12)	0.0061(2)	0	0	0
Cu	0.0067(2)	0.0067(2)	0.0056(3)	0.00145(16)	0.00145(16)	-0.0002(2)
Ga	0.0040(3)	0.0047(3)	0.0139(3)	0	0	0
M	0.0296(5)	0.0032(3)	0.0073(3)	0	0	0

similar structures) were used to locate them in the structure. Position 8*f* is occupied by the copper atoms, the Ga atoms are located in 8*i*, and a statistical mixture *M* (0.25Cu+0.75Ga) is situated in 8*j*. For comparison, results of the structural investigation of the $YbCu_{5.4}Ga_{6.6}$ phase can be found in [21].

The unit cell and the coordination polyhedra of the atoms in $YbCu_5Ga_7$ are displayed in Fig. 1*b*. The values of the interatomic distances (Table 5) are in good agreement with the sums of the atomic radii of the respective components. The Yb atoms are situated inside 20-vertex pseudo Frank-Kasper polyhedra. The closest Yb–Cu/Ga/*M* contacts range from 2.986(1) to 3.304(1) Å. The neighbors of the Cu and *M* atoms form deformed icosahedra. 14-vertex Frank-Kasper polyhedra surround the Ga atoms. The shortest contact distances are 2.561(1) Å (Cu–Cu), 2.640(1) Å (Cu–Ga), 2.642(1) Å (Ga–Ga), 2.525(1) Å (Ga–*M*), and 2.600(1) Å (*M*–*M*).

The structure type $ThMn_{12}$ is well described in the literature, and there exist many reports on different binary and ternary representatives [13]. It is structurally related to the $CaCu_5$ structure type, and can be obtained by partial substitution of the large Ca atoms by pairs of smaller ones along the *c*-axis: $2(RT_5) - R + 2T \rightarrow RT_{12}$. The relations between the lattice parameters of these two structure types are: $a(ThMn_{12}) \sim 2c(CaCu_5)$ and $c(ThMn_{12}) \sim a(CaCu_5)$. Replacement of all the large atoms by smaller atoms leads to the Zr_4Al_3 structure type, the relationship between these structures being displayed in Fig. 3. There are many structures with general formula

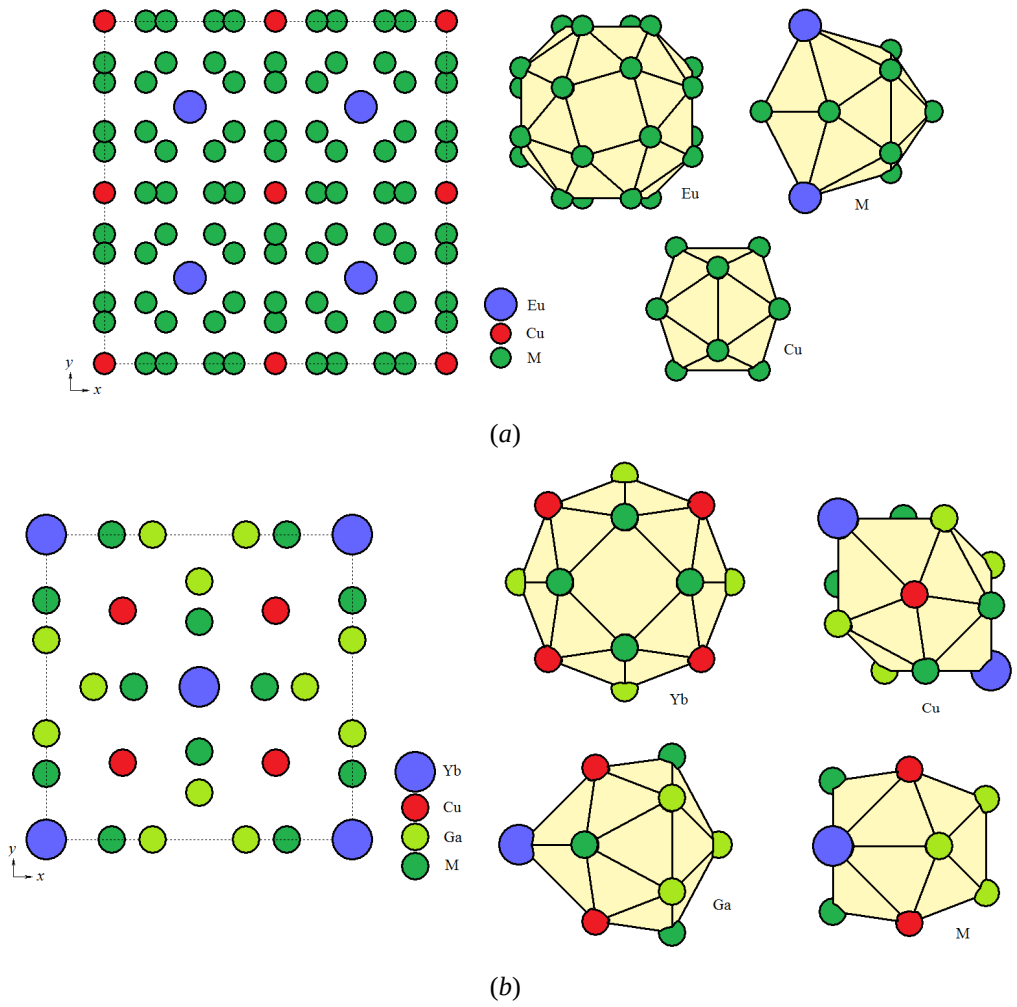

Fig. 1 The unit cell and the coordination polyhedra of the atoms in the structures of the $EuCu_8Ga_5$ (*a*) and $YbCu_5Ga_7$ (*b*) phases.

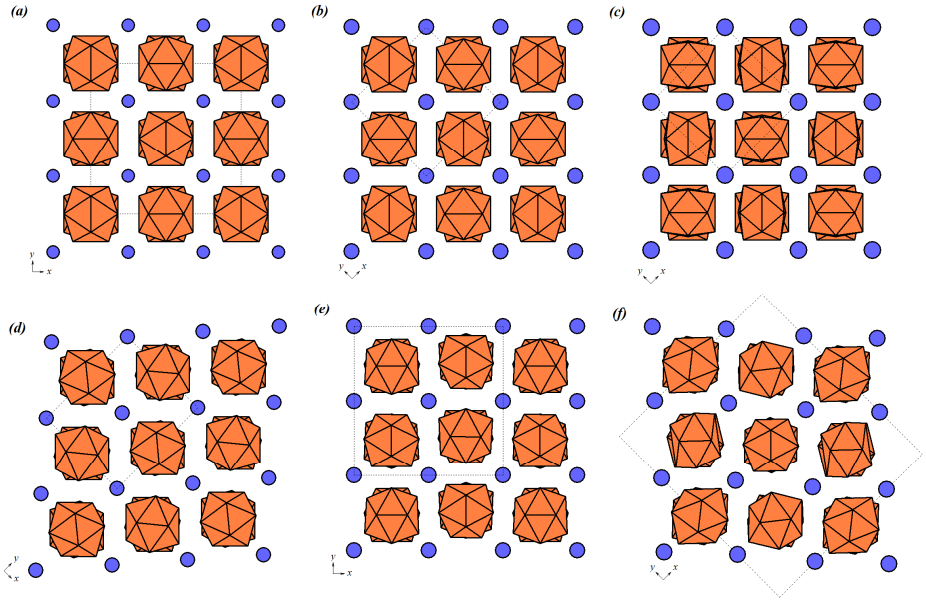

Fig. 2 The crystal structures of $NaZn_{13}$ (*a*), $CeNi_{8.5}Si_{4.5}$ (*b*), $SrNi_{6.3}Si_{6.7}$ (*c*), $LaNi_{7.36}In_{5.64}$ (*d*), $SrCu_7In_6$ (*e*), $SrNi_{7.9}In_{5.1}$ (*f*). The unit cells are marked by dotted lines. Alkaline, alkaline earth, and rare earth metals are shown by blue circles. The icosahedra formed by *d*- and *p*-metals are displayed by orange color.

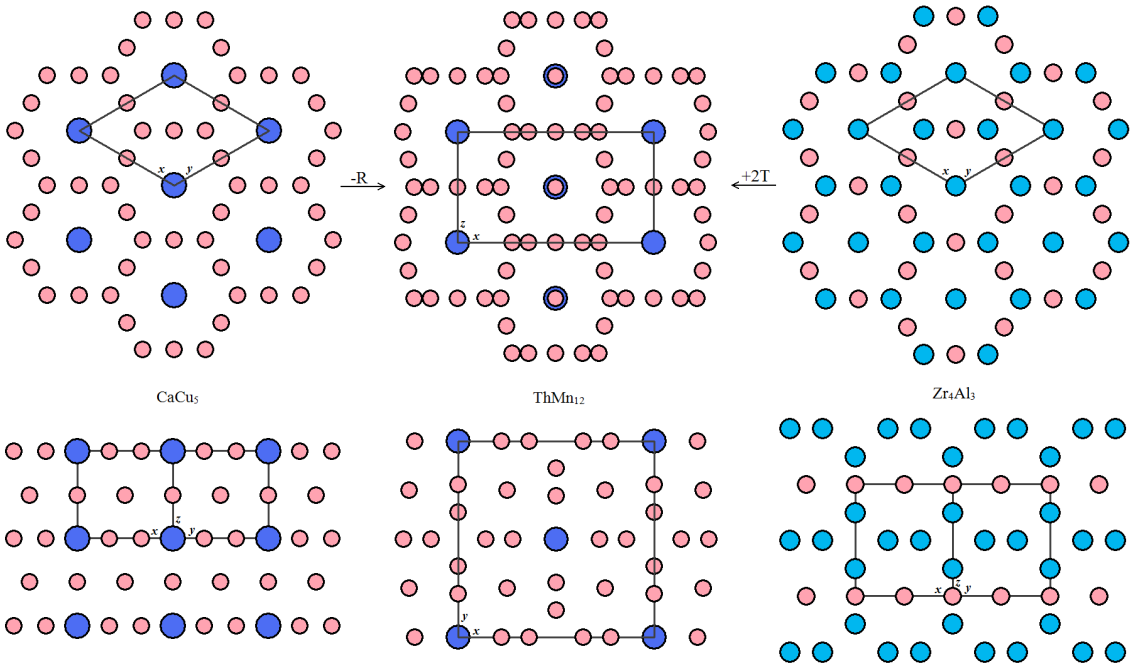

Fig. 3 Relationship between the structure types $CaCu_5$, Zr_4Al_3, and $ThMn_{12}$.

$R_{1-x}T_{5+2x}$, with x from 0 ($CaCu_5$-type) to 1 (Zr_4Al_3-type). For example, structures with ordered substitution of the atoms are Ce_3Zn_{22} (x = 1/4, $4(RT_5) - R + 2T \rightarrow R_3T_{22}$), Th_2Ni_{17} and Th_2Zn_{17} (x = 1/3, $3(RT_5) - R + 2T \rightarrow R_2T_{17}$), $TiBe_{12}$, $LiFe_6Ge_6$, and $ScNi_6Ge_6$ (x = 1/2, $2(RT_5) - R + 2T \rightarrow RT_{12}$); structures with disordered substitution of the atoms are $TbCu_7$ (x = 0.22), UZn_{12} (x = 0.27), $SmZn_{12}$ (x = 0.44), *etc*. [16,22].

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