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The new monoclinic structure type Gd_4ReGe_8

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A new monoclinic structure type of intermetallic compounds, Gd_4ReGe_8 ($mP64$-12, $P2_1/c$, a = 5.8106(7), b = 16.060(2), c = 12.852(2) Å, β = 115.379(9)°, R = 0.0405, R_w = 0.0866), was identified on the basis of X-ray single-crystal diffraction data. The structure of Gd_4ReGe_8 is a monoclinic derivative of the $CeNiSi_2$ type, formed as a result of partial ordering of *d*-element vacancies. The structure, which contains four partly occupied Re sites, is closely related to the Tb_4FeGe_8 type, where only two partly occupied Fe sites were refined.

Gadolinium / Rhenium / Germanium / Bärnighausen formalism / X-ray diffraction

Introduction

The structure type $CeNiSi_2$ [1] is a common type of intermetallic compounds. The major part of the compounds (90) form in systems R–T–Ge, where R = 4*f*-element, T = *d*-element [2]. Several superstructures of the $CeNiSi_2$ type are also known in these systems, such as: $LuMnGe_2$ [3], $YIrGe_2$ [4], $Ce_2Rh_{1.35}Ge_{4.65}$ [5], Tb_4FeGe_8 [6], *etc*. There exist also information about compounds isotypic with the structure types $ZrSi_2$ [7] and $ErGe_{2.16}$ [8], which are defect, binary variants of the structure type $CeNiSi_2$. Compounds with $CeNiSi_2$-type structures are known in the systems R–{Cr, Ru, Co, Cu}–Ge, whereas the ternary germanides of osmium belong to the structure types $ZrCrSi_2$ [9] and $YIrGe_2$ [4]. Many ternary compounds in the systems R–{Mn, Re, Fe, Rh, Ir, Ni, Pd, Pt}–Ge adopt the $CeNiSi_2$ type, or one of its superstructure. On the contrary, compounds with $CeNiSi_2$-type structures, or superstructures of it, have not been observed in R–T–Ge systems where T = Ti, Zr, Hf, V, Nb, Ta, Mo, W, Ag, Au, Zn, Cd, or Hg.

The overwhelming majority of the compounds that crystallize in the $CeNiSi_2$ type is characterized by defects on the position of the T-element. For a particular T-element, the amount of vacancies decreases with increasing periodic number of the R-element. This is due to the size factor, whereas differences in deficiency within the series of compounds with the same rare-earth element and different *d*-elements, may be attributed to electronic factors (*e.g.* number of valence electrons).

The synthesis and structural investigation of a new compound forming in the system Gd–Re–Ge were the aim of this paper.

Experimental details

Alloys were synthesized from high-purity elements (≥ 99.7 wt.%) by arc melting on a water-cooled copper bottom under a purified (using Ti as a getter) argon atmosphere with a tungsten electrode. The alloys were placed into an alumina crucible and inserted into a Ta ampoule, which was then sealed by welding under Ar atmosphere. The samples were heated to 1350°C in a vacuum tube furnace at the speed of 200°C/h, kept at constant temperature for 5 h and then cooled down to room temperature at a cooling rate of 50°C/h. The weight losses during the preparation of the samples were about 1 % of the total mass, which was 1 g for each alloy.

A single crystal was extracted from one of the alloys. It was mounted on a glass fiber and X-ray diffraction data were collected at room temperature on an Xcalibur diffractometer (Mo $K\alpha$-radiation, λ = 0.71073 Å, CCD detector). The structure of Gd_4ReGe_8 was solved by direct methods in the space group $P2_1/c$ with the SHELXS-97 program [10,11]. The thermal oscillations of the atoms were described by anisotropic displacement parameters.

Table 1 Experimental details and crystallographic data for the compound Gd_4ReGe_8.

Empirical formula	$Gd_4Re_{0.991(8)}Ge_8$
Chemical formula weight M, g·mol^{-1}	1395.92
Pearson symbol, Z	mP64-12, 4
Crystal system, space group	monoclinic, $P2_1/c$
Unit-cell parameters: a, Å	5.8106(7)
b, Å	16.060(2)
c, Å	12.852(2)
β, °	115.379(9)
Unit-cell volume V, Å^3	1083.6(3)
Density D_X, g·cm^{-3}	8.556
$F(000)$	2348
Diffractometer	Xcalibur Onyx
Radiation, monochromator	Mo $K\alpha$, graphite
Absorption correction	analytical
Absorption coefficient μ, mm^{-1}	56.972
Extinction coefficient	0.00028(2)
Weighing scheme	$w = 1/[\sigma^2(F_o^2)+(0.019P)^2+57.85P]$, where $P = (F_o^2+2F_c^2)/3$
Limiting indices	$-5 \leq h \leq 5$, $-20 \leq k \leq 20$, $-16 \leq l \leq 16$
θ_{min}-θ_{max}, °	4.6-26.3
Number of reflections: measured / unique / with $F > 2\sigma(F)$	20089 / 2021 / 1887
Size of the crystal, mm	0.09 × 0.04 × 0.04
Color of the crystal	gray
Number of refined parameters	131
Reliability factors: R	0.0405
R_w	0.0866
χ^2	1.173

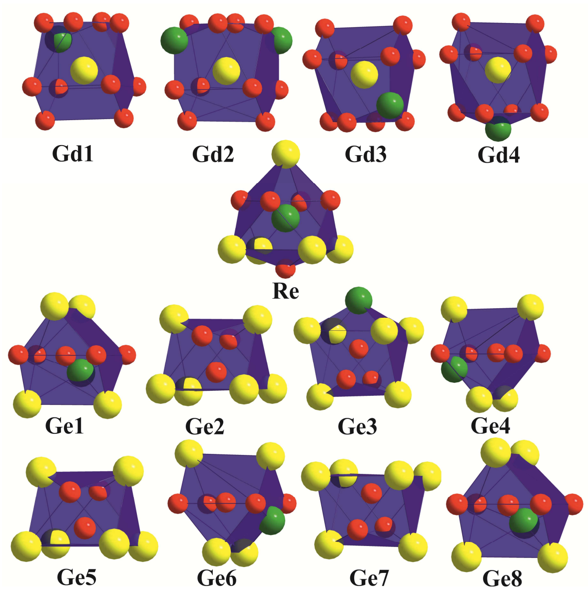


Fig. 1 Coordination polyhedra of the atoms in the structure of Gd_4ReGe_8. The sites with <5 % occupation are ignored.

Because of the partial occupancies of the Re sites, the displacement parameters were constrained to be equal. Full-matrix least-squares refinements of the positional and anisotropic displacement parameters were performed on F^2 using the SHELXL-97 program.

Details of the data collection and structure refinement for Gd_4ReGe_8 are given in Table 1. The coordinates and equivalent displacement parameters of the atoms in the structure of Gd_4ReGe_8 are listed in Table 2, and the anisotropic displacement parameters in Table 3. The coordination polyhedra are shown on Fig. 1.

Table 2 Atomic coordinates, equivalent displacement parameters and site occupancies for Gd_4ReGe_8, space group $P2_1/c$.

Atom	Wyckoff position	x	y	z	Occ.	U_{eq}, Å^2
Gd1	4e	0.05953(13)	0.10009(4)	0.43430(6)	1	0.0096(2)
Gd2	4e	0.31290(13)	0.10298(4)	0.18816(6)	1	0.0107(2)
Gd3	4e	0.56641(13)	0.39883(4)	0.44145(6)	1	0.0098(2)
Gd4	4e	0.81161(13)	0.39195(4)	0.18627(6)	1	0.0112(2)
Re1	4e	0.066(13)	0.293(4)	0.428(5)	0.008(2)	0.0098(2)
Re2	4e	0.18611(11)	0.69791(3)	0.31155(5)	0.916(4)	
Re3	4e	0.318(3)	0.3044(10)	0.1857(14)	0.0322(16)	
Re4	4e	0.562(3)	0.2008(9)	0.4335(13)	0.0345(16)	
Ge1	4e	0.0434(3)	0.74867(9)	0.45261(13)	1	0.0144(4)
Ge2	4e	0.0634(3)	0.44663(9)	0.43841(12)	1	0.0123(3)
Ge3	4e	0.1855(3)	0.54385(9)	0.31188(12)	1	0.0109(3)
Ge4	4e	0.2299(3)	0.25174(9)	0.32864(13)	1	0.0148(4)
Ge5	4e	0.3139(3)	0.44346(9)	0.18579(12)	1	0.0125(3)
Ge6	4e	0.3968(3)	0.25208(9)	0.04870(13)	1	0.0143(4)
Ge7	4e	0.4393(3)	0.54946(9)	0.06523(12)	1	0.0122(3)
Ge8	4e	0.6734(3)	0.24886(9)	0.33061(13)	1	0.0155(4)

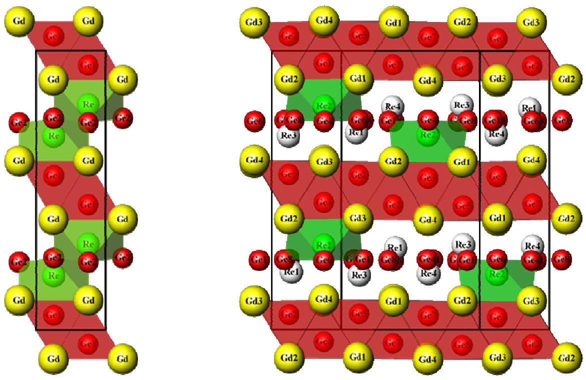
Table 3 Anisotropic displacement parameters (Å^2) for Gd_4ReGe_8.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Gd1	0.0089(4)	0.0099(3)	0.0103(4)	-0.0018(2)	0.0045(3)	-0.0013(2)
Gd2	0.0105(4)	0.0112(3)	0.0106(4)	-0.0018(2)	0.0046(3)	-0.0010(3)
Gd3	0.0088(4)	0.0100(3)	0.0109(4)	0.0014(2)	0.0046(3)	0.0016(2)
Gd4	0.0109(4)	0.0112(3)	0.0116(4)	0.0009(2)	0.0049(3)	0.0008(3)
Re1-Re4	0.0084(4)	0.0101(3)	0.0109(3)	0.0006(2)	0.0043(2)	0.0004(2)
Ge1	0.0123(8)	0.0134(7)	0.0172(8)	-0.0018(6)	0.0061(6)	0.0010(6)
Ge2	0.0094(8)	0.0161(7)	0.0121(7)	-0.0006(6)	0.0052(6)	0.0027(6)
Ge3	0.0106(7)	0.0129(7)	0.0101(7)	-0.0002(5)	0.0055(6)	0.0021(6)
Ge4	0.0166(9)	0.0151(7)	0.0144(8)	-0.0016(6)	0.0084(6)	-0.0037(6)
Ge5	0.0090(8)	0.0193(7)	0.0099(7)	-0.0019(6)	0.0048(6)	0.0026(6)
Ge6	0.0150(8)	0.0133(7)	0.0158(8)	0.0004(6)	0.0077(6)	0.0011(6)
Ge7	0.0104(8)	0.0158(7)	0.0114(7)	-0.0017(6)	0.0054(6)	0.0024(6)
Ge8	0.0128(8)	0.0150(7)	0.0155(8)	-0.0018(6)	0.0030(6)	0.0014(6)

Results and discussion

Investigations of compounds forming in the systems *R*–Re–Ge can be found in [12-15]. Three compounds with the $CeNiSi_2$-type structures have been reported in these systems: $GdRe_{0.24-0.25}Ge_2$, $HoRe_{0.25}Ge_2$, and $LuRe_{0.12}Ge_2$. During a systematic investigation of the {Gd, Er}–Re–Ge systems we found a new compound with Er and confirmed the existence of the phase with Gd, as well in as-cast alloys as in samples annealed at 800°C [13]. No single crystals could be isolated and the structures were refined by the powder method. After a slightly modified synthesis (slow heating and cooling), a crystal suitable for X-ray single crystal diffraction was found. Examining the structure of the Gd-compound, we found a new monoclinic derivative of the $CeNiSi_2$ type.

The crystal structure of the $CeNiSi_2$ type contains layers of square antiprisms (fragments of $BaAl_4$-type structure or its ternary variant $CeAl_2Ga_2$) and layers of trigonal prisms (fragment of AlB_2-type structure), which alternate along the *y*-axis in the ratio 1:1. Similar fragments were found in the new structure type Gd_4ReGe_8 (Fig. 2). In both structures the square antiprisms and trigonal prisms are connected by common faces, but in the structure of $CeNiSi_2$ two neighboring antiprisms, shifted by ½ perpendicular to the *z*-axis, share edges. In the structure of Gd_4ReGe_8 neighboring antiprisms with more than 5 % occupation of the central site are separated.



$CeNiSi_2$ (*Cmcm*) Gd_4ReGe_8 (*P*2_1/*c*)

Fig. 2 Comparison of the structure types $CeNiSi_2$ and Gd_4ReGe_8.

The unit cell of the new structure type can be derived from that of the parent structure $CeNiSi_2$ (see Table 4, blue square on Fig. 3). The partial ordering of 75 % vacancies on the *d*-element site is accompanied by a four-time increase of the cell, and by a decrease in symmetry. The transformation can be described using the Bärnighausen formalism (group-subgroup relations). The first operation considered here is the elimination of the side-centering of the Bravais lattice, which leads to space group *Pbnm* and releases the constraints on the *x*-coordinates (model II). At the next step the symmetry is decreased to the monoclinic space group *P*2_1/*n*, which implies release of the constraints on the *z*-coordinates (model III). Standardization to space group setting *P*2_1/*c* (model III', red parallelogram on Fig. 3) changes only the cell parameters (the new parameter *a* is former *c*, and the new parameter *c* is the diagonal between the old parameters *c* and *a*). Only four of the original symmetry elements remain in this monoclinic structure. The next operation consists in increasing the cell by a factor 2 along the *x*-axis, by that doubling the number of independent atom sites, a first time (model IV, green parallelogram on Fig. 3), and then once more (model V, yellow parallelogram on Fig. 3). At this step, there are 16 atom sites in Wyckoff position 4*e*: four for Gd atoms, four for Re atoms and eight for Ge atoms. The last operation is again a standardization to space group setting *P*2_1/*c* (model V', violet parallelogram on Fig. 3).

Table 4 Transformation from the structure type $CeNiSi_2$ (compound $GdRe_{0.25}Ge_2$) to the structure type Gd_4ReGe_8.

Model	**I $CeNiSi_2$**	**II**	**III**	**III'**
Group-subgroup relation		IIa	I	0
Transformation matrix		1 0 0 0 1 0 0 0 1	1 0 0 0 1 0 0 0 1	0 0 1 0 1 0 -1 0 -1
Space group	(63) *Cmcm*	(62) *Pbnm*	(14) $P2_1/n$	(14) $P2_1/c$
Unit-cell parameters, Å	$a_{\mathrm{I}} = 4.1571$ $b_{\mathrm{I}} = 16.0583$ $c_{\mathrm{I}} = 4.0543$	$a_{\mathrm{II}} = 4.1571$ $b_{\mathrm{II}} = 16.0583$ $c_{\mathrm{II}} = 4.0543$	$a_{\mathrm{III}} = 4.1571$ $b_{\mathrm{III}} = 16.0583$ $c_{\mathrm{III}} = 4.0543$ $\beta_{\mathrm{III}} = 90.0°$	$a_{\mathrm{III'}} = 4.0543$ $b_{\mathrm{III'}} = 16.0583$ $c_{\mathrm{III'}} = 5.8068$ $\beta_{\mathrm{III'}} = 134.28°$
Atom, Wyckoff position, coordinates	Gd 4*c* 0, 0.3990, ¼ Re[a] 4*c* 0, 0.1980, ¼ Ge1 4*c* 0, 0.0501, ¼ Ge2 4*c* 0, 0.7501, ¼	Gd 4*c* 0.0, 0.3990, ¼ Re[a] 4*c* 0.0, 0.1980, ¼ Ge1 4*c* 0.0, 0.0501, ¼ Ge2 4*c* 0.0, 0.7501, ¼	Gd 4*e* 0.0, 0.3990, 0.25 Re[a] 4*e* 0.0, 0.1980, 0.25 Ge1 4*e* 0.0, 0.0501, 0.25 Ge2 4*e* 0.0, 0.7501, 0.25	Gd 4*e* 0.25, 0.3990, 0.0 Re[a] 4*e* 0.25, 0.1980, 0.0 Ge1 4*e* 0.25, 0.0501, 0.0 Ge2 4*e* 0.25, 0.7501, 0.0
Symmetry elements	1, 2, 2, 2, -1, *m*, *c*, *m*, *t*, 2, 2, 2, -1, *n*, *n*, *b*	1, 2, ~~2, 2,~~ -1, *m*, ~~*c*, *m*, *t*, 2,~~ 2, 2, ~~-1, *n*,~~ *n*, *b*	1, ~~2, 2, 2,~~ -1, *m*, ~~*c*, *m*, *t*, 2,~~ 2, ~~2, -1, *n*,~~ *n*, ~~*b*~~	1, 2, -1, *c*

Model	**IV**	**V**	**V' Gd_4ReGe_8**
Group-subgroup relation	IIc	IIc	0
Transformation matrix	0 0 2 0 1 0 -1 0 -1	0 0 4 0 1 0 -1 0 -1	-1 0 -1 0 -1 0 -1 0 3
Space group	(14) $P2_1/c$	(14) $P2_1/n$	(14) $P2_1/c$
Unit-cell parameters, Å	$a_{\mathrm{IV}} = 8.1086$ $b_{\mathrm{IV}} = 16.0583$ $c_{\mathrm{IV}} = 5.8068$ $\beta_{\mathrm{IV}} = 134.28°$	$a_{\mathrm{V}} = 16.2172$ $b_{\mathrm{V}} = 16.0583$ $c_{\mathrm{V}} = 5.8068$ $\beta_{\mathrm{V}} = 134.28°$	$a_{\mathrm{V'}} = 5.8068$ $b_{\mathrm{V'}} = 16.0583$ $c_{\mathrm{V'}} = 12.8537$ $\beta_{\mathrm{V'}} = 115.41°$
Atom, Wyckoff position, coordinates	Gd1 4*e* 0.125, 0.3990, 0.0	Gd1 4*e* 0.0625, 0.3990, 0.0	Gd1 4*e* 0.0625, 0.1010, 0.4375
		Gd2 4*e* 0.5625, 0.3990, 0.0	Gd2 4*e* 0.5625, 0.3990, 0.4375
	Gd2 4*e* 0.625, 0.3990, 0.0	Gd3 4*e* 0.3125, 0.3990, 0.0	Gd3 4*e* 0.3125, 0.1010, 0.1875
		Gd4 4*e* 0.8125, 0.3990, 0.0	Gd4 4*e* 0.8125, 0.3990, 0.1875
	Re1[a] 4*e* 0.125, 0.1980, 0.0	Re1[a] 4*e* 0.0625, 0.1980, 0.0	Re1 4*e* 0.0625, 0.3020, 0.4375
		Re2[a] 4*e* 0.5625, 0.1980, 0.0	Re2 4*e* 0.5625, 0.1980, 0.4375
	Re2[a] 4*e* 0.625, 0.1980, 0.0	Re3[a] 4*e* 0.3125, 0.1980, 0.0	Re3 4*e* 0.3125, 0.3020, 0.1875
		Re4[a] 4*e* 0.8125, 0.1980, 0.0	Re4 4*e* 0.8125, 0.1980, 0.1875
	Ge1 4*e* 0.125, 0.0501, 0.0	Ge1 4*e* 0.0625, 0.0501, 0.0	Ge1 4*e* 0.0625, 0.4499, 0.4375
		Ge2 4*e* 0.5625, 0.0501, 0.0	Ge2 4*e* 0.5625, 0.0501, 0.4375
	Ge2 4*e* 0.625, 0.0501, 0.0	Ge3 4*e* 0.3125, 0.0501, 0.0	Ge3 4*e* 0.3125, 0.4499, 0.1875
		Ge4 4*e* 0.8125, 0.0501, 0.0	Ge4 4*e* 0.8125, 0.0501, 0.1875
	Ge3 4*e* 0.125, 0.7501, 0.0	Ge5 4*e* 0.0625, 0.7501, 0.0	Ge5 4*e* 0.0625, 0.7499, 0.4375
		Ge6 4*e* 0.5625, 0.7501, 0.0	Ge6 4*e* 0.5625, 0.7501, 0.4375
	Ge4 4*e* 0.625, 0.7501, 0.0	Ge7 4*e* 0.3125, 0.7501, 0.0	Ge7 4*e* 0.3125, 0.7499, 0.1875
		Ge8 4*e* 0.8125, 0.7501, 0.0	Ge8 4*e* 0.8125, 0.7501, 0.1875
Symmetry elements	1, 2, -1, *c*	1, 2, -1, *n*	1, 2, -1, *c*

[a] Occ. = 0.25.

I CeNiSi$_2$ ($Cmcm$; **a**, **b**, **c**)
–IIa→
model II ($Pbnm$; **a**, **b**, **c**)
–I→
model III ($P2_1/n$; **a**, **b**, **c**)
–0→
model III' ($P2_1/c$; **c**, **b**, **-a-c**)
–IIc→
model IV ($P2_1/c$; **2c**, **b**, **-a-c**)
–IIc→
model V ($P2_1/n$; **4c**, **b**, **-a-c**)
–0→
V' Gd$_4$ReGe$_8$ ($P2_1/c$; **-a-c**, **-b**, **-a+3c**)

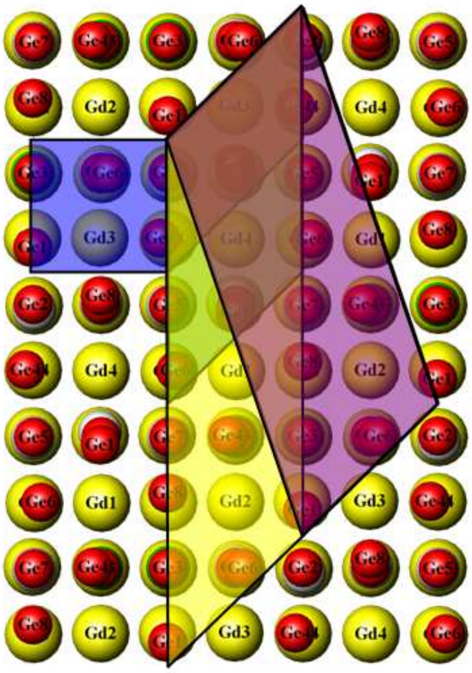


Fig. 3 Transformation from the structure type $CeNiSi_2$ to the structure type Gd_4ReGe_8 (blue cell: I $CeNiSi_2$, models II and III, red cell: model III', green cell: model IV, yellow cell: model V, violet cell: V' Gd_4ReGe_8).

Table 5 Comparison of the atomic coordinates of the theoretical and experimental structures of Gd_4ReGe_8 (space group $P2_1/c$).

Atom	$x_{theor.}$	$x_{exp.}$	$y_{theor.}$	$y_{exp.}$	$z_{theor.}$	$z_{exp.}$
Gd1	0.0625	0.05953(13)	0.1010	0.10009(4)	0.4375	0.43430(6)
Gd2	0.3125	0.31290(13)	0.1010	0.10298(4)	0.1875	0.18816(6)
Gd3	0.5625	0.56641(13)	0.3990	0.39883(4)	0.4375	0.44145(6)
Gd4	0.8125	0.81161(13)	0.3990	0.39195(4)	0.1875	0.18627(6)
Re1	0.0625	0.066(13)	0.3020	0.293(4)	0.4375	0.428(5)
Re2	0.1875	0.18611(11)	0.6980	0.69791(3)	0.3125	0.31155(5)
Re3	0.3125	0.318(3)	0.3020	0.3044(10)	0.1875	0.1857(14)
Re4	0.5625	0.562(3)	0.1980	0.2008(9)	0.4375	0.4335(13)
Ge1	0.0625	0.0434(3)	0.7499	0.74867(9)	0.4375	0.45261(13)
Ge2	0.0625	0.0634(3)	0.4499	0.44663(9)	0.4375	0.43841(12)
Ge3	0.1875	0.1855(3)	0.5501	0.54385(9)	0.3125	0.31188(12)
Ge4	0.1875	0.2299(3)	0.2501	0.25174(9)	0.3125	0.32864(13)
Ge5	0.3125	0.3139(3)	0.4499	0.44346(9)	0.1875	0.18579(12)
Ge6	0.4375	0.3968(3)	0.2501	0.25208(9)	0.0625	0.04870(13)
Ge7	0.4375	0.4393(3)	0.5501	0.54946(9)	0.0625	0.06523(12)
Ge8	0.6875	0.6734(3)	0.2499	0.24886(9)	0.3125	0.33061(13)

The atomic coordinates of the theoretical and experimental structures are compared in Table 5. Selected interatomic distances are listed in Table 6.

All of the four *d*-element positions derived from the parent type $CeNiSi_2$ are present in Gd_4ReGe_8, even if the occupation of three of them is very low. However, only two positions exist in the related structure type Tb_4FeGe_8 [6]. In the case of Gd_4ReGe_8, removal of any of the partly occupied Re sites from the refinement led to significantly worse reliability factors. The coordinates and occupancies of the atom sites in the structures of Gd_4ReGe_8 and Tb_4FeGe_8 are presented in Table 7.

The coordination polyhedra of the atoms in Gd_4ReGe_8 are related to those of the $CeNiSi_2$ type and can be described as follows: Gd[Ge_8] square prisms with three or four additional atoms, Re[Ge_4Gd_4] square antiprisms with two additional atoms, Ge[Gd_6] trigonal prisms with two or three additional atoms, and Ge[Gd_4Ge_4] *gyrobifastigia* (two trigonal prisms, rotated by 90° with respect to each other and sharing a square face) with one additional atom.

The crystal structure of the Gd_4ReGe_8 compound can also be represented as a packing of Gd-centered polyhedra formed by Ge atoms. The Re atoms occupy square pyramidal voids in the packing (Fig. 4).

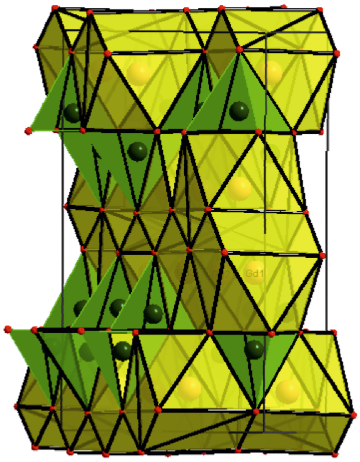


Fig. 4 Packing of Gd-centered polyhedra in the structure of Gd_4ReGe_8 (small red circles: Ge atoms, medium green circles: Re atoms, large yellow circles: Gd atoms).

Conclusions

The crystal structure of the new ternary germanide Gd_4ReGe_8 represents a new structure type (Pearson symbol *mP*64-12, space group $P2_1/c$). Ignoring Re sites with <5 % occupation, the coordination polyhedra are square prisms with three or four additional atoms for Gd, square antiprisms with two additional atoms for Re, and trigonal prisms with two or three additional atoms, and *gyrobifastigia* with one additional atom for Ge. The crystal structure can also be represented as a packing of Gd-centered polyhedra formed by Ge atoms, with Re atoms in voids.

The structure of Gd_4ReGe_8 can be derived from the $CeNiSi_2$ type by removing ¾ of the *d*-element atoms and both structure types consequently contain the same basic fragments. Partial ordering of the vacancies causes lowering of the symmetry from orthorhombic to monoclinic and an increase of the cell volume by a factor 4.

The crystal structure of Gd_4ReGe_8 is closely related to the structure type Tb_4FeGe_8, where only two of the four *d*-element sites present in Gd_4ReGe_8 are occupied.

Table 6 Interatomic distances and coordination numbers in the structure of Gd_4ReGe_8. Distances to the sites with <5 % occupation are ignored.

Atoms		*δ*, Å	CN	Atoms		*δ*, Å	CN
Gd1	Ge3	2.999(12)	11	Gd2	Ge7	2.991(13)	12
	Ge5	3.004(13)			Ge2	3.008(13)	
	Ge7	3.013(2)			Ge3	3.048(2)	
	Ge1	3.019(3)			Ge3	3.066(2)	
	Ge7	3.021(2)			Ge1	3.134(10)	
	Ge6	3.028(8)			Ge6	3.152(3)	
	Ge4	3.148(4)			Ge8	3.153(10)	
	Ge8	3.155(8)			Ge4	3.154(3)	
	Ge7	3.207(10)			Ge2	3.269(9)	
	Ge5	3.248(9)			Re2	3.277(1)	
	Re2	3.259(11)			Re2	3.285(1)	
					Ge5	3.298(9)	
Gd3	Ge8	2.996(3)	11	Gd4	Ge5	3.005(2)	11
	Ge2	3.004(2)			Ge5	3.036(2)	
	Ge2	3.006(2)			Ge2	3.058(13)	
	Ge3	3.010(12)			Ge7	3.069(13)	
	Ge4	3.013(8)			Re2	3.116(1)	
	Ge5	3.055(13)			Ge3	3.205(9)	
	Ge6	3.148(4)			Ge6	3.214(11)	
	Ge3	3.152(10)			Ge1	3.237(4)	
	Ge1	3.156(8)			Ge4	3.242(11)	
	Ge2	3.213(9)			Ge7	3.258(9)	
	Re2	3.263(11)			Ge8	3.263(4)	

Table 6 (*continued*)

Atoms		δ, Å	CN	Atoms		δ, Å	CN
Ge1	Re2	2.435(5)	9	Ge2	Ge3	2.564(4)	8
	Ge6	2.551(3)			Ge2	2.643(4)	
	Ge8	2.558(15)			Gd3	3.004(2)	
	Gd1	3.019(3)			Gd3	3.006(2)	
	Gd2	3.134(10)			Gd2	3.008(13)	
	Gd3	3.156(8)			Gd4	3.058(13)	
	Gd4	3.237(4)			Gd3	3.213(9)	
	Ge6	3.261(3)			Gd2	3.269(9)	
	Ge4	3.266(2)					
Ge3	Re2	2.474(2)	9	Ge4	Re2	2.471(14)	9
	Ge2	2.564(4)			Ge6	2.567(9)	
	Ge5	2.611(5)			Ge8	2.567(3)	
	Gd1	2.999(12)			Gd3	3.013(8)	
	Gd3	3.010(12)			Gd1	3.148(4)	
	Gd2	3.048(2)			Gd2	3.154(3)	
	Gd2	3.066(2)			Gd4	3.242(11)	
	Gd3	3.152(10)			Ge8	3.245(3)	
	Gd4	3.205(9)			Ge1	3.266(2)	
Ge5	Ge7	2.607(4)	8	Ge6	Re2	2.475(14)	9
	Ge3	2.611(5)			Ge1	2.551(3)	
	Gd1	3.004(13)			Ge4	2.567(9)	
	Gd4	3.005(2)			Gd1	3.028(8)	
	Gd4	3.036(2)			Gd3	3.148(4)	
	Gd3	3.055(13)			Gd2	3.152(3)	
	Gd1	3.248(9)			Gd4	3.214(11)	
	Gd2	3.298(9)			Ge1	3.261(3)	
					Ge8	3.274(2)	
Ge7	Ge5	2.607(4)	8	Ge8	Re2	2.440(5)	9
	Ge7	2.617(4)			Ge1	2.558(15)	
	Gd2	2.991(13)			Ge4	2.567(3)	
	Gd1	3.013(2)			Gd3	2.996(3)	
	Gd1	3.021(2)			Gd2	3.153(10)	
	Gd4	3.069(13)			Gd1	3.155(8)	
	Gd1	3.207(10)			Ge4	3.245(3)	
	Gd4	3.258(9)			Gd4	3.263(4)	
					Ge6	3.274(2)	
Re2	Ge1	2.435(5)	10				
	Ge8	2.440(5)					
	Ge4	2.471(14)					
	Ge3	2.474(2)					
	Ge6	2.475(14)					
	Gd4	3.116(1)					
	Gd1	3.259(11)					
	Gd3	3.263(11)					
	Gd2	3.277(1)					
	Gd2	3.285(1)					

Table 7 Positional coordinates and occupancies of the atom sites in the structures of Gd_4ReGe_8 (this work) and Tb_4FeGe_8 [6] (space group $P2_1/c$, all atoms in Wyckoff position 4*e*).

Gd_4ReGe_8					Tb_4FeGe_8				
Atom	*x*	*y*	*z*	Occ.	Atom	*x*	*y*	*z*	Occ.
Re1	0.066(13)	0.293(4)	0.428(5)	0.008(2)	–				
Re2	0.18611(11)	0.69791(3)	0.31155(5)	0.916(4)	Fe1	0.1881	0.6977	0.3128	0.8
Re3	0.318(3)	0.3044(10)	0.1857(14)	0.0322(16)	–				
Re4	0.562(3)	0.2008(9)	0.4335(13)	0.0345(16)	Fe2	0.5662	0.1971	0.4392	0.2

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