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Interaction of the components in the Gd–Ni–Sn ternary system at 770 K

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ABSTRACT

The phase equilibria in the Gd–Ni–Sn ternary system were determined at 770 K by means of X-ray and metallographic analyses in the whole concentration range. The Gd–Ni–Sn system is characterized by formation of 14 ternary intermetallic compounds: $GdNi_{4.89}Sn$ ($CeCu_{4.38}In_{1.62}$-type), $Gd_{12}Ni_6Sn$ ($Sm_{12}Ni_6In$-type), Gd_6Ni_2Sn (Ho_6Co_2Ga-type), Gd_2Ni_2Sn (W_2CoB_2-type), GdNiSn (TiNiSi-type), $Gd_2Ni_7Sn_3$ ($Dy_2Ni_7Sn_3$-type), $Gd_3Ni_8Sn_4$ ($Lu_3Co_{7.77}Sn_4$-type), $GdNi_3Sn_2$ ($HoNi_{2.6}Ga_{2.4}$-type), $GdNi_2Sn_2$ ($LaPt_2Ge_2$-type), $GdNiSn_2$ ($LuNiSn_2$-type), $Gd_3Ni_4Sn_6$ ($Ce_3Pd_4Sn_6$-type), $Gd_{40}Ni_{15}Sn_{45}$ (structure unknown), $GdNi_{2.67}Sn_{5.44}$ ($GdNi_{2.67}Sn_{5.44}$-type), and $GdNiSn_4$ ($LuNiSn_4$-type). The crystal chemistry analysis of ternary compounds formed in the Gd–Ni–Sn system was done.

1. Introduction

The Ni-containing ternary systems with rare earth metals (R) and tin were not studied completely until the present. A contribution to the investigation into R–Ni–Sn systems has been made by our research team with the study of the phase equilibria for Ce–Ni–Sn [1], Nd–Ni–Sn [2], Dy–Ni–Sn [3], and Lu–Ni–Sn [4] ternary systems. The phase relations in the Y–Ni–Sn system were partly investigated (up to 50 at.% of Sn content) and briefly described in Ref. [5]. Recently, the La–Ni–Sn system was studied by Zhuang et al. [6].

The rest of the R–Ni–Sn ternary systems were studied with the aim to find some isostructural series of the compounds and investigating their crystallographic and physical parameters. The investigated systems are characterized by a large number of the ternary stannides that are crystallized with well-known and its own structure types. The Ni-rich corner of the R–Ni–Sn phase diagrams is the more complicated and characterized by the ternary phases with the structures derivatives of $CaCu_5$-type. The *f*-element contribution to the chemical and structural characteristics of ternary phases generates different structure types in this part of R–Ni–Sn systems passing from light rare earths to heavy rare earth elements, but all of them content the fragment of $CaCu_5$-type—$CeNi_5Sn$-type (RNi_5Sn, R = La–Nd) [7], $CeCu_{4.38}In_{1.62}$-type (RNi_5Sn, R = Sm, Gd–Yb) [8], $Dy_2Ni_7Sn_3$-type [9], $HoCo_{2.6}Ga_{2.4}$-type (RNi_3Sn_2, R = Y, Sm, Gd, Tb) [10], $YbNi_{2-x}Sn$ [11] and $Lu_3Co_{7.77}Sn_4$-type ($R_3Ni_8Sn_4$, R = Sm, Gd) [12].

The preliminary information about Gd–Ni–Sn ternary system at 770 K (0–50 at.% Sn) and 670 K (more than 50 at.% Sn) was reported in Ref. [5], but the phase equilibria were not presented. The most compounds we found and studied earlier during the investigation of isotypic series of ternary compounds formed in R–Ni–Sn systems and crystallographic parameters for them are gathered in Ref. [5]. With regard to the work in progress on the R–Ni–Sn ternary systems and new ternary stannides, it was decided to perform the detailed study the Gd–Ni–Sn system at 770 K, especially in Ni-rich region.

2. Binary boundary systems

The binary boundary Gd–Sn, Gd–Ni and Ni–Sn systems have been investigated earlier and their phase diagrams are well known in the literature; they are briefly described in the following.

2.1. Ni–Sn system

The version of this well-known phase diagram, used here is taken from Massalski [13] and Villars [14]. In the system three phases are observed: Ni_3Sn (own type), Ni_3Sn_2 (low-temperature phase, own type), Ni_3Sn_4 (own type). The peritectoid formation of the NiSn phase at 873 K was reported in Ref. [15].

2.2. Gd–Sn system

The data concerning the Gd–Sn binary system were used according to Refs. [5,13,14]. Six phases form at 770 K: Gd_5Sn_3 (Mn_5Si_3-type), Gd_5Sn_4 (Sm_5Ge_4-type), $Gd_{11}Sn_{10}$ ($Ho_{11}Ge_{10}$-type), $GdSn_2$ ($ZrSi_2$-type), Gd_3Sn_7 (own type), $GdSn_{2.75}$ (own type). The

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Table 1
Crystallographic characteristics of the compounds in the Gd–Ni–Sn ternary system.

No.[a]	Compound	Structure type	Space group	Lattice parameters (nm)		
				a	*b*	*c*
1	$Gd_{12}Ni_6Sn$	$Sm_{12}Ni_6In$	*Im*−3*m*	0.99406(2)	–	–
2	Gd_6Ni_2Sn	Ho_6Co_2Ga	*Immm*	0.9480(4)	0.9658(6)	1.0023(3)
3	$GdNi_{4.89}Sn$	$CeCu_{4.38}In_{1.62}$	*Pnnm*	1.60369(1)	1.01807(1)	0.48464(1)
4	Gd_2Ni_2Sn	W_2CoB_2	*Immm*	0.4294(1)	0.5638(1)	0.8390(1)
5	$Gd_2Ni_7Sn_3$	$Dy_2Ni_7Sn_3$	*Cmca*	0.86341(5)	2.3779(1)	0.75553(5)
6	$Gd_3Ni_8Sn_4$	$Lu_3Co_{7.77}Sn_4$	*P*6$_3$*mc*	0.89003(2)	–	0.74711(5)
7	$GdNi_3Sn_2$	$HoGa_{2.4}Ni_{2.6}$	*P*6/*mmm*	0.91858(4)	–	0.42670(2)
8	GdNiSn	TiNiSi	*Pnma*	0.7236(3)	0.4461(1)	0.7676(4)
9	$GdNi_2Sn_2$	$LaPt_2Ge_2$	*P*12$_1$1	0.4367(4) $\beta = 90.223(5)^\circ$	0.4365(4)	0.9700(8)
10	$Gd_3Ni_4Sn_6$	$Ce_3Pd_4Sn_6$	*Pnma*	1.5221(4)	0.4361(5)	1.4406(3)
11	$Gd_{40}Ni_{15}Sn_{45}$			Structure unknown		
12	$GdNiSn_2$	$LuNiSn_2$	*Pnma*	1.60628(8)	0.44325(2)	1.4672(7)
13	$GdNi_{2.67}Sn_{5.44}$	$GdNi_{2.67}Sn_{5.44}$	*Im*−3	1.1854(6)	–	–
14	$GdNiSn_4$	$LuNiSn_4$	*Ammm*	0.4410(1)	2.8325(3)	0.4369(1)

[a] The compounds number corresponds to the figures in the phase diagram (Fig. 1).

existence of high temperature phase $GdSn_3$ with cubic Cu_3Au-type was reported in Ref. [16].

2.3. Gd–Ni system

The phase diagram as assessed by Massalski [13] and Villars [14] has been taken for our investigation. Nine binary phases are formed at 770 K in the Gd–Ni system: Gd_2Ni_{17} (Th_2Ni_{17}-type), $GdNi_5$ ($CaCu_5$-type), $GdNi_4$ (structure unknown), Gd_2Ni_7 (Ce_2Ni_7-type), $GdNi_3$ ($PuNi_3$-type), $GdNi_2$ ($MgCu_2$-type), GdNi (TlI-type), Gd_3Ni_2 (structure unknown), and Gd_3Ni (CFe_3-type).

3. Experimental

The samples were prepared by a repeated arc melting of the constituent elements (gadolinium with a purity of 99.8 wt.%, nickel—99.99 wt.%, tin—99.99 wt.%) under high purity Ti-gettered argon atmosphere on a water-cooled copper crucible. The weight losses of the initial total mass were lower than 1 wt.%. The alloys were annealed at 770 K in evacuated silica tubes for 1 month and quenched in cold water.

Phase analysis was performed using X-ray powder diffraction of the synthesized samples (RKD-57 with CrK radiation and DRON-2.0M with FeK_α radiation). The observed diffraction intensities were compared with reference powder patterns of binary and known ternary phases. The compositions of the obtained samples were examined by Scanning Electron Microscopy (SEM) using JEOL-840A scanning microscope. Quantitative electron probe microanalysis (EPMA) of the phases was carried out using an energy-dispersive X-ray analyser with the pure elements as standards (an acceleration voltage was 20 kV; *K*- and *L*-lines were used). The data for the crystal structure refinements were collected at room temperature using HZG-4a (CuK_α radiation), STOE STADI P ($CuK_{\alpha1}$ radiation) and Bruker D8 diffractometers (graphite monochromator, $CuK_{\alpha1}$ radiation, 20–100° 2θ range with scanning step 0.02° and 20 s exposure time). Calculations of the unit cell parameters and theoretical patterns were performed using the CSD [17] and WinPLOTR [18] program packages.

4. Results and discussion

The phase equilibria in the Gd–Ni–Sn ternary system have been established at 770 K using X-ray analysis of 215 ternary and binary alloys. The isothermal sections of this system are presented in Fig. 1. The microphotographs of some alloys are shown in Fig. 2. The Gd–Ni–Sn system is characterized by the formation of 14 ternary compounds crystallographic characteristics of which are listed in Table 1.

The presence of almost all binary compounds in the Gd–Sn and Ni–Sn systems corresponding to the reference data was confirmed. To check the existence of the NiSn binary stannide [15] the several alloys of closed compositions were prepared and annealed at 770 K, 870 K, and 1070 K. Phase analysis of the corresponding samples showed the presence of two phases—Ni_3Sn_4 and Ni_3Sn_2 at all investigated temperatures. In the Gd–Ni binary system we have synthesized all the samples with the stoichiometry corresponding to the literature data. Phase analysis of the corresponding samples confirmed a formation of Gd_2Ni_{17} (Th_2Ni_{17}-type), $GdNi_5$ ($CaCu_5$-type), Gd_2Ni_7 (Ce_2Ni_7-type), $GdNi_3$ ($PuNi_3$-type), $GdNi_2$ ($MgCu_2$-type), GdNi (TlI-type), and Gd_3Ni (CFe_3-type) binaries. The powder patterns of alloys at $GdNi_4$ and Gd_3Ni_2 stoichiometry content two phases: $GdNi_5 + Gd_2Ni_7$ and $GdNi + Gd_3Ni$, respectively.

A formation of interstitial solid solutions based on the RSn_2 (R = Gd–Lu) series of binary compounds with $ZrSi_2$ structure was reported in Refs. [19,20] and was confirmed for Gd during investigations of Gd–Ni–Sn system. The Ni solubility in the $GdSn_2$ ($ZrSi_2$-type) binary compound is equal to 7 at.%, and the solid solution has a direction toward the $GdNiSn_2$ compound. The volume of the unit cell of the solid solution samples increases with increasing of the nickel content in the alloys confirming the formation of the solid solution formed by insertion of nickel atoms into the $GdSn_2$ structure and can be described using $GdNi_xSn_2$ formula (Table 2). The formation of the $GdNi_{5-x}Sn_x$ solid solution formed by substitution of the nickel atoms by tin in $GdNi_5$ ($CaCu_5$-type) up to 5 at.% Sn was found. The compositions and values of the lattice parameters are given in Table 3.

The existence of the earlier known Gd_6Ni_2Sn (Ho_6Co_2Ga-type) [21], $Gd_{12}Ni_6Sn$ ($Sm_{12}Ni_6In$-type) [22], $GdNi_5Sn$ ($CeCu_{4.38}In_{1.62}$-type) [8], $GdNi_3Sn_2$ ($HoNi_{2.6}Ga_{2.4}$-type) [10], $GdNi_2Sn_2$ ($CaBe_2Ge_2$-type) [5], $GdNiSn_2$ ($LuNiSn_2$-type) [23], GdNiSn (TiNiSi-type) [24],

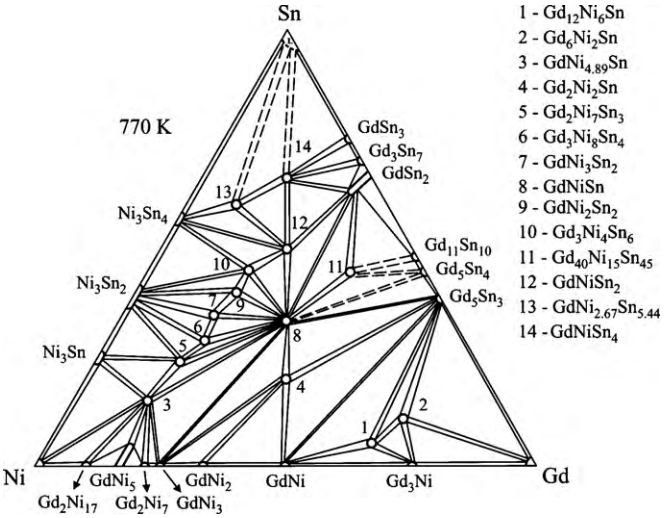

Fig. 1. Isothermal section of the Gd–Ni–Sn phase diagram at 770 K.

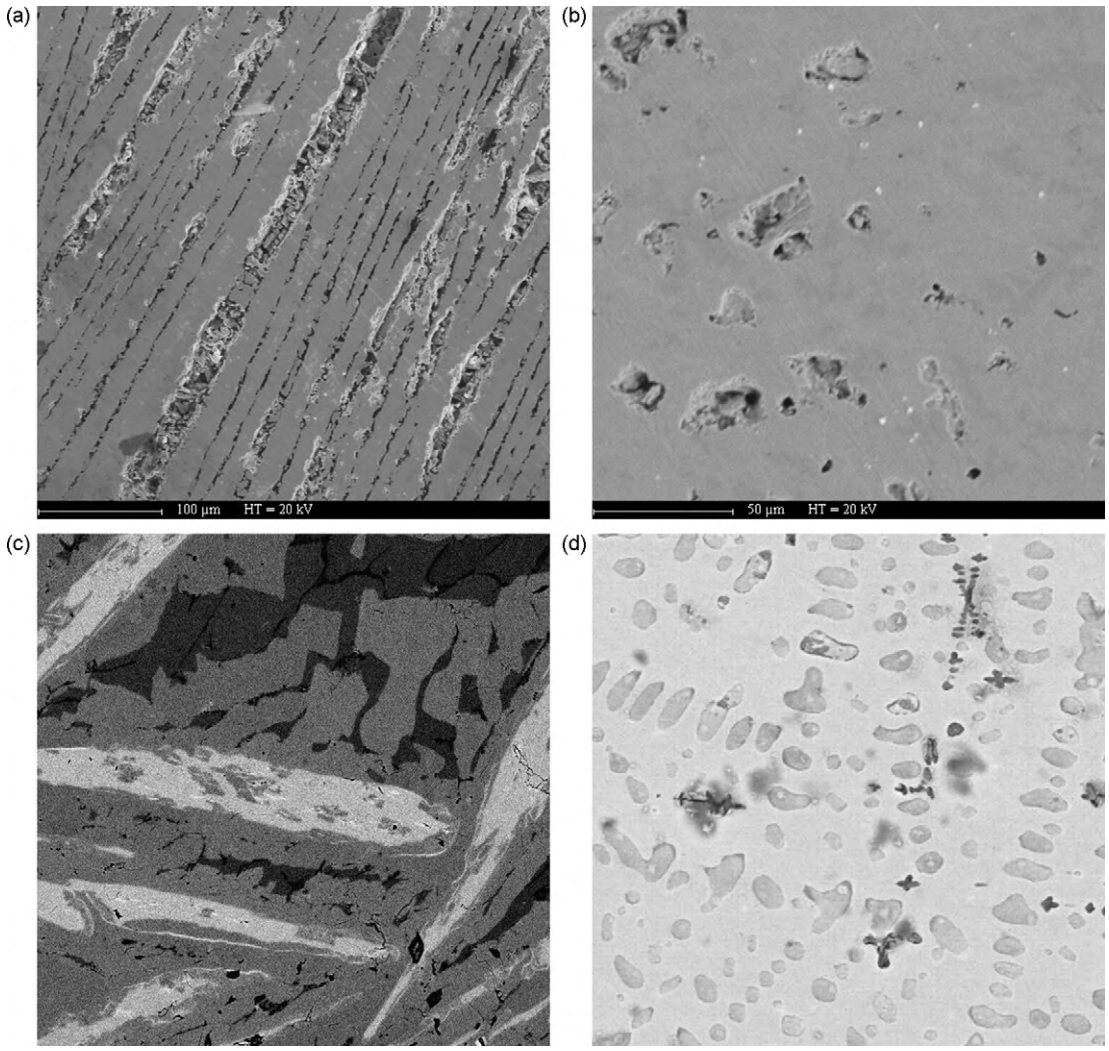

Fig. 2. Electron micrographs of the alloys: (a) $Gd_{17}Ni_{20}Sn_{63}$–$GdNiSn_4$ (gray phase); $GdNiSn_2$ (white phase); $GdNi_{2.67}Sn_{5.44}$ (black phase); (b) $Gd_{10}Ni_{30}Sn_{60}$–$GdNi_{2.67}Sn_{5.44}$ (gray phase); (c) $Gd_{15}Ni_{50}Sn_{35}$–$GdNi_3Sn_2$ (gray dark phase); $GdNi_2Sn_2$ (gray light phase); Ni_3Sn_2 (black phase); (d) $Gd_{63}Ni_{27}Sn_{10}$–$Gd_{12}Ni_6Sn$ (gray light phase); Gd_5Sn_3 (gray phase).

$GdNi_{2.67}Sn_{5.44}$ (own structure type) [25], Gd_2Ni_2Sn (W_2CoB_2-type) [26], and $GdNiSn_4$ ($LuNiSn_4$-type) [27] compounds was confirmed and new ternary stannides were found: $Gd_3Ni_8Sn_4$, $Gd_2Ni_7Sn_3$, $Gd_3Ni_4Sn_6$, and $\sim Gd_{45}Ni_{15}Sn_{40}$.

By the results of X-ray analysis of the samples in the Ni-rich part of the Gd–Ni–Sn system two new ternary compounds at compositions $Gd_{15}Ni_{65}Sn_{20}$ and $Gd_{20}Ni_{53}Sn_{27}$ were found. The powder pattern of the $Gd_{20}Ni_{53}Sn_{27}$ sample was indexed on the basis of the hexagonal lattice with cell parameters $a = 0.89003(2)$ nm, $c = 0.74711(5)$ nm, and indicated that this compound belongs to the $Lu_3Co_{7.77}Sn_8$ type structure (space group $P6_3mc$). The crystal structure of $Gd_3Ni_8Sn_4$ compound was determined using X-ray powder diffraction method (HZG-4a, WinPLOTR package). Refined atomic coordinates and displacement parameters are listed in Table 4. The observed, calculated and difference X-ray patterns of $Gd_{20}Ni_{53}Sn_{27}$ sample are shown in Fig. 3. The analysis of the structure showed that interatomic distances Gd–Sn1 (0.3176 nm), Ni2–Ni4 (0.2413 nm), and Ni–Sn (0.2520 nm) are shorter than the sum of the respective atomic radii. The $Gd_2Ni_7Sn_3$ compound formed at $Gd_{15}Ni_{65}Sn_{20}$ composition was found to be isostructural to the previously studied $Dy_2Ni_7Sn_3$ compound crystallized in own structure type (space group *Cmca*) [9] with the lattice parameters $a = 0.86341(5)$ nm, $b = 2.3779(1)$ nm, $c = 0.75553(5)$ nm.

Table 2
Composition and lattice parameters of the samples of the $GdNi_xSn_2$ solid solution.

Composition	Lattice parameters (nm)			V (nm^3)
	a	b	c	
$Gd_{33}Sn_{67}$[a]	0.4428	1.6410	0.4322	0.3141
$Gd_{33}Ni_2Sn_{65}$[a]	0.4429(8)	1.649(2)	0.4331(2)	0.3163
$Gd_{32}Ni_5Sn_{63}$[a]	0.4431(9)	1.658(1)	0.4343(1)	0.3191
$Gd_{31}Ni_7Sn_{62}$[a]	0.4433(9)	1.667(1)	0.4357(2)	0.3219
$Gd_{30}Ni_{10}Sn_{60}$[b]	0.4434(7)	1.667(1)	0.4359(3)	0.3221

[a] Single phase sample.
[b] Two phase sample.

Table 3
Composition and lattice parameters of the samples of the $GdNi_{5-x}Sn_x$ solid solution.

Composition	Lattice parameters (nm)			V (nm^3)
	a	b	c	
$Gd_{17}Ni_{83}$[a]	0.4907(3)	–	0.3965(3)	0.08156
$Gd_{17}Ni_{81}Sn_2$[a]	0.4872(1)	–	0.3973(1)	0.08167
$Gd_{17}Ni_{78}Sn_5$[a]	0.4943(4)	–	0.3968(4)	0.08180
$Gd_{17}Ni_{76}Sn_7$[b]	0.4944(5)	–	0.3968(2)	0.08180

[a] Single phase sample.
[b] Two phase sample.

Table 4
Atomic positional and isotropic displacement parameters for the $Gd_3Ni_8Sn_4$ compound (R_p = 0.0185, R_{wp} = 0.0235, R_{Bragg} = 0.1030).

Atom	Wyckoff position	*x*/*a*	*y*/*b*	*z*/*c*	$B_{iso} \times 10^2$ (nm^2)
Gd	6*c*	0.47533(7)	0.52467(7)	0	1.03(4)
Ni1	6*c*	0.8364(6)	0.1635(6)	0.8360(10)	0.76(5)
Ni2	6*c*	0.8936(2)	0.1063(2)	0.5228(11)	0.76(5)
Ni3	2*b*	1/3	2/3	0.6831(17)	0.76(5)
Ni4	2*a*	0	0	0.2860(14)	0.76(5)
Sn1	6*c*	0.8295(2)	0.1704(2)	0.2110(6)	0.27(2)
Sn2	2*b*	1/3	2/3	0.3236(7)	0.27(2)

The crystal structure of the $GdNi_2Sn_2$ compound was refined during our investigation by powder method (Bruker D8, WinPLOTR package). According to Ref. [5] this compound crystallizes in the $CaBe_2Ge_2$ structure type (SG *P*4/*nmm*) with unit cell parameters *a* = 0.4369(5) nm, *c* = 0.9709(3) nm, but the structure refinements using this starting model were not satisfactory. Previous investigation of isotypic $CeNi_2Sn_2$ compound showed two polymorphic modifications—tetragonal with $CaBe_2Ge_2$-type and monoclinic one with $LaPt_2Ge_2$-type [5,28]. Thus, for further crystal structure calculations of $GdNi_2Sn_2$ the starting model of the monoclinic $LaPt_2Ge_2$ structure was chosen. The powder pattern reflections of the $GdNi_2Sn_2$ phase were well indexed in $P12_11$ space group with lattice parameters *a* = 0.43674(4) nm, *b* = 0.43650(4) nm, *c* = 0.97005(8) nm, β = 90.223(5)°. However, the sample contains some phase/phases which were not identified due to the rather high background and low quality of diffraction pattern. To confirm the model of the structure, the single crystal investigation of this compound is carrying out.

The existence of the $GdNiSn_2$ compound and its lattice parameters were reported earlier [23]. During present work, the crystal structure of this stannide was refined by X-ray powder diffraction method (HZG-4a, WinPLOTR package). The $GdNiSn_2$ compound crystallizes in the $LuNiSn_2$-type structure (space group *Pnma*, *a* = 1.60628(8) nm, *b* = 0.44325(2) nm, *c* = 1.46727(7) nm) with the atomic parameters presented in Table 5. The observed, calculated and difference X-ray patterns of the $GdNiSn_2$ compound are shown in Fig. 4.

The detailed crystal structure refinements performed on $Gd_{15}Ni_{70}Sn_{15}$ sample confirmed a formation of $GdNi_5Sn$ compound with $CeCu_{4.38}In_{1.62}$-type (space group *Pnnm*, *a* = 1.60369(1) nm, *b* = 1.01807(1) nm, *c* = 0.48464(1) nm). The refinements of the site occupancies showed that two 4*g* positions for Ni1 and Ni2 atoms are occupied by 89% and 88%, respectively. Thus, the chemical formula of the compound should be written as $GdNi_{4.89}Sn$. The atomic parameters are presented in Table 6, the observed, calculated and difference X-ray patterns of the $GdNi_{4.89}Sn$ compound are shown in Fig. 5.

Table 5
Atomic positional and isotropic displacement parameters for the $GdNiSn_2$ compound (R_{Bragg} = 0.114, R_p = 0.027, R_{wp} = 0.034).

Atom	Wyckoff position	*x*/*a*	*y*/*b*	*z*/*c*	B_{iso}[a] $\times 10^2$ (nm^2)
Gd1	4*c*	0.8488(9)	1/4	0.5273(1)	0.40(1)
Gd2	4*c*	0.3757(9)	1/4	0.2325(9)	0.40(1)
Gd3	4*c*	0.1439(8)	1/4	0.1101(1)	0.40(1)
Ni1	4*c*	0.5504(2)	1/4	0.8933(2)	0.64(9)
Ni2	4*c*	0.8027(2)	1/4	0.7484(2)	0.64(9)
Ni3	4*c*	0.2941(2)	1/4	0.4547(2)	0.64(9)
Sn1	4*c*	0.1842(9)	1/4	0.3308(1)	0.49(8)
Sn2	4*c*	0.4516(1)	1/4	0.4512(1)	0.49(8)
Sn3	4*c*	0.0223(1)	1/4	0.4187(1)	0.49(8)
Sn4	4*c*	0.7147(9)	1/4	0.8866(2)	0.49(8)
Sn5	4*c*	0.9611(1)	1/4	0.7551(1)	0.49(8)
Sn6	4*c*	0.6687(1)	1/4	0.6230(1)	0.49(8)

[a] The isotropic displacement parameters were constrained for each atomic element.

According to Ref. [5] the Gd–Ni–Sn system is characterized by the formation of two ternary compounds with ~$Gd_{20}Ni_{35}Sn_{45}$ and ~$Gd_{25}Ni_{32}Sn_{43}$ compositions. By the results of X-ray and metallographic analyses of the corresponding samples we have found that above mentioned phases in fact represent only one ternary compound at $Gd_{23}Ni_{32}Sn_{45}$ composition with $Ce_3Pd_4Sn_6$ structure type (space group *Pnma*, *a* = 1.5221(4) nm, *b* = 0.4361(5) nm, *c* = 1.4406(3) nm).

All ternary compounds in the Gd–Ni–Sn ternary system are characterized by narrow homogeneity ranges at investigated temperature.

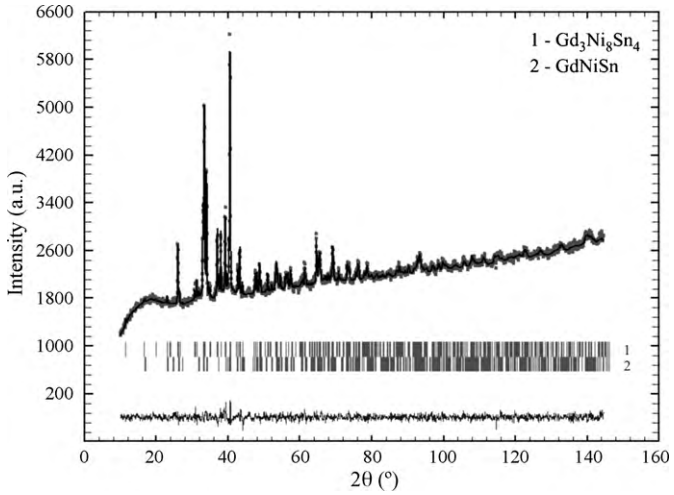

Fig. 3. The observed, calculated and difference X-ray patterns of $Gd_{20}Ni_{53}Sn_{27}$ sample.

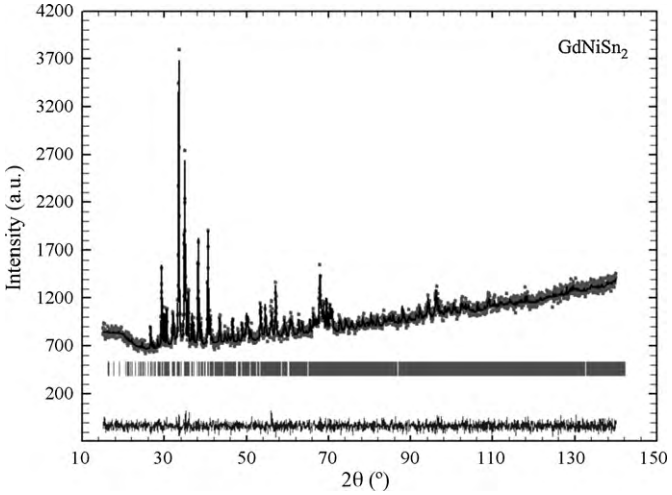

Fig. 4. The observed, calculated and difference X-ray patterns of the $GdNiSn_2$ compound.

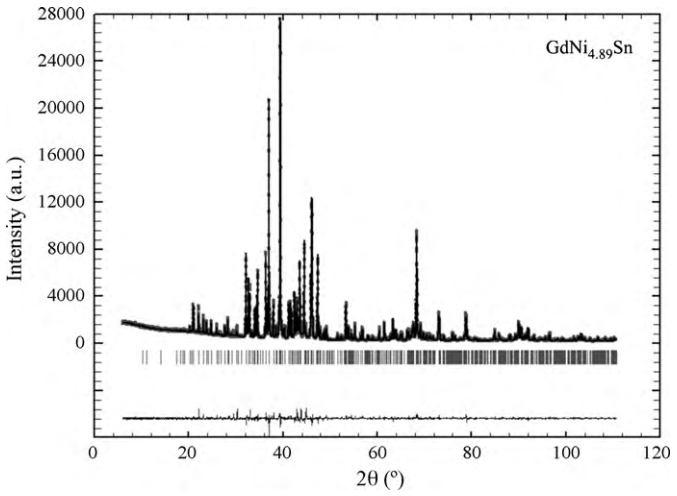

Fig. 5. The observed, calculated and difference X-ray patterns of the $GdNi_{4.89}Sn$ compound.

The crystal chemistry analysis of ternary compounds formed in the Gd–Ni–Sn system showed that they could be divided into several groups based on the structural fragments of several binary compounds: $GdSn_2$ ($ZrSi_2$-type), $GdNi_5$ ($CaCu_5$-type), Gd_3Ni (Fe_3C-type) as presented in Fig. 6. Previously we performed the crystal chemistry analysis for compounds formed in the Dy–Ni–Sn ternary system [3]. The studied Gd–Ni–Sn system is characterized by the presence of higher number of intermediate phases and this fact allowed us to complete our classification, especially for derivatives of $CaCu_5$-type and Fe_3C-type. The GdNiSn compound belongs to TiNiSi structure type and is a derivative of $Gd_{11}Sn_{10}$ binary stannide ($Ho_{11}Ge_{10}$-type). According to the systemic the covalence contribution in the ternary compounds of $ZrSi_2$-type group decreases with the increasing distance from appropriate ternary stannide to the $GdSn_2$. The compounds that belong to $CaCu_5$-type group are characterized by strong Ni–Ni interaction and large coordinate numbers for Gd atoms. The compounds of Fe_3C-type group are characterized by short Gd–Ni and Gd-Gd distances.

In conclusion the Gd–Ni–Sn ternary system is characterized by more complicated character of the phase relations which take place in the series of the R–Ni–Sn systems where R—La, Ce, Nd, Dy and Lu, investigated for the present time. The existence of 14 ternary phases in this system is a result of the interaction between the components in all parts of the diagram. The similarity in the interaction of the components in all investigated systems is displayed by the formation of compound with the equiatomic composition in the whole rare earth elements crystallizing with the TiNiSi structure type, and the formation of $RNiSn_2$ ($CeNiSi_2$ and $LuNiSn_2$-types) and RNi_5Sn series compounds ($CeNi_5Sn$-type and $CeCu_{4.38}In_{1.62}$-type). Comparing the present study of the Gd–Ni–Sn system and data reported in Ref. [5] we may note a formation 14 ternary phases at 770 K. The more remarkable difference is related to the Ni- and Sn-rich parts of Gd–Ni–Sn system, where two new $Gd_3Ni_8Sn_4$ and $Gd_2Ni_7Sn_3$ phases were found, and the existence of $\sim Gd_2NiSn_7$ was not confirmed, respectively.

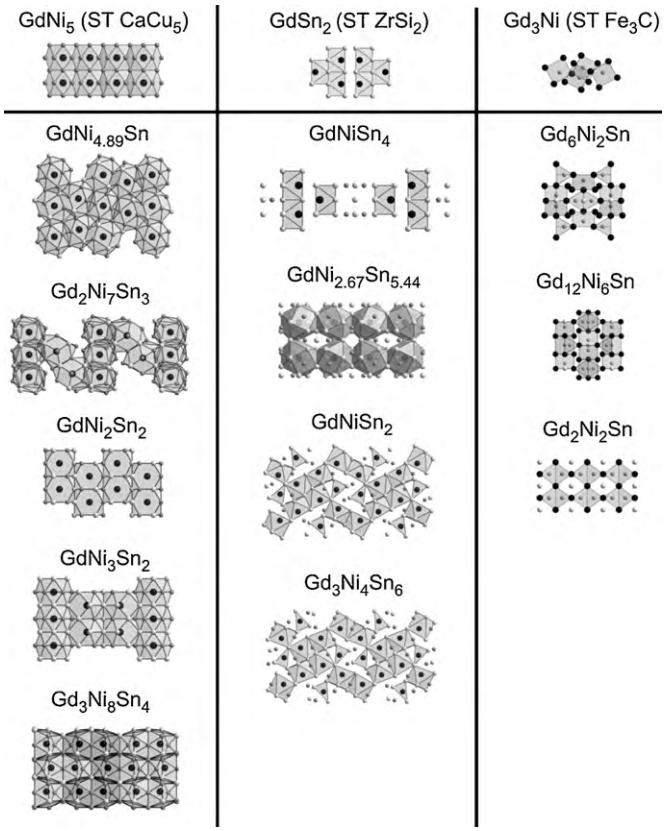

Fig. 6. Distribution of compounds by the similarity of the structures in the Gd–Ni–Sn system.

Table 6
Atomic and isotropic displacement parameters for the $GdNi_{4.89}Sn$ compound ($R_{Bragg} = 0.047$, $R_p = 0.056$, $R_{wp} = 0.082$).

Atom	Wyckoff position	*x*/*a*	*y*/*b*	*z*/*c*	B_{iso}[a] × 10^2 (nm^2)
Gd1	2*a*	0	0	0	0.19(6)
Gd2	2*d*	1/2	0	0	0.19(6)
Gd3	4*g*	0.7508(1)	0.3835(2)	0	0.19(6)
Ni1[b]	4*g*	0.2195(4)	0.2972(6)	0	0.25(2)
Ni2[b]	4*g*	0.5843(4)	0.4559(6)	0	0.25(2)
Ni3	4*g*	0.4668(4)	0.3080(6)	0	1.32(1)
Ni4	4*g*	0.3984(4)	0.1509(6)	0	1.32(1)
Ni5	4*g*	0.1721(3)	0.0730(6)	0	1.32(1)
Ni6	4*g*	0.1007(4)	0.4608(7)	0	1.32(1)
Ni7	8*h*	0.5923(2)	0.2545(4)	0.2472(8)	1.33(1)
Ni8	8*h*	0.8424(3)	0.1351(4)	0.2520(7)	1.33(1)
Sn1	4*g*	0.9478(2)	0.3022(2)	0	1.13(9)
Sn2	4*g*	0.6945(1)	0.0851(2)	0	1.13(9)

[a] The isotropic displacement parameters were constrained for each atomic element.
[b] Occupation: Ni1 = 0.89(1); Ni2 = 0.88(1).

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