

Crystal structure and hydrogenation properties of the hexagonal Dy_2M_{17} and $Dy_2M_{17}C_x$ ($M = Fe, Co, Ni; x < 0.5$) compounds

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The crystal structures of the Dy_2M_{17} ($M = Fe, Co, Ni$) compounds were investigated from single crystal X-ray diffraction data (Th_2Ni_{17} type structure, space group $P6_3/mmc$). The Dy_2M_{17} binaries ($M = Co, Ni$) dissolve limited amounts of carbon, up to 0.2 ($M = Co$) and 0.4 ($M = Ni$) at. C/f.u. The hydrogenation properties of the parent compounds and their carbides were investigated. Dy_2M_{17} ($M = Co, Ni$) absorb 3.4 ($M = Co$) and 3.5 ($M = Ni$) at. H/f.u. at 5 MPa hydrogen pressure. The carbides $Dy_2M_{17}C_x$ ($M = Co, Ni$) absorb 2.7 ($M = Co$) and 2.8 ($M = Ni$) at. H/f.u. The synthesized carbides, hydrides and carbohydrides preserve the crystal structure of the parent compounds.

Hydrides / Carbides / Crystal structure / X-ray diffraction

Introduction

Intermetallic rare-earth (R) and 3d-transition-metal-rich compounds R_2M_{17} ($M = Fe, Co, Ni$) are widely known in science and technology for their unique physical properties [1]. A distinctive feature of these compounds is their ability to considerably change their properties upon introduction of light element atoms (H, N or C) into voids of the crystal lattice.

Most of the R_2M_{17} ($M = Fe, Co, Ni$) compounds crystallize in hexagonal Th_2Ni_{17} -type or rhombohedral Th_2Zn_{17} -type structures [2,3]. These two structure types are derived from the $CaCu_5$ (RM_5) parent type by replacement of part of the large atoms (R) by pairs of small atoms ($M-M$). Since the composition can deviate from the ideal R_2M_{17} stoichiometry and since the degree of disorder is known to depend on the method of preparation, special attention is paid to the substitution rate of the rare-earth atoms during the structure refinements [2-5].

Among the family of R_2M_{17} and related compounds, the R_2Fe_{17} compounds and their carbides $R_2Fe_{17}C_x$ and hydrides $R_2Fe_{17}H_x$ are the most studied compounds as promising materials for permanent magnets. They exhibit large magnetic moments originating from the 3d sublattice and magnetocrystalline anisotropy arising from the rare-

earth sublattice. On account of the different atomic radii, two different types of structure are observed for binary R_2Fe_{17} compounds: the rhombohedral Th_2Zn_{17} and the hexagonal Th_2Ni_{17} [3,6] type. For example, for Dy_2Fe_{17} Buschow reported a Th_2Ni_{17} -type structure for samples annealed at 1000°C [3]. In this structure the Dy atoms occupy the (2b) and (2d) sites, while the Fe atoms occupy (4f), (6g), (12j), and (12k) positions. Depending on the preparation conditions and the Dy:Fe stoichiometry, in addition to the Th_2Ni_{17} -type structure a Th_2Zn_{17} -type structure may form [6]. The as-cast, stoichiometric sample was single-phase with Th_2Ni_{17} structure, whereas in off-stoichiometric samples, annealed at 1050°C, a mixture of Th_2Ni_{17} - and Th_2Zn_{17} -type structures was observed. The amount of Th_2Zn_{17} -type structure increased with increasing Dy content [6]. The investigation of the crystal structure of Dy_2Fe_{17} by means of X-ray single crystal diffraction [7] indicated small deviations from 2:17 stoichiometry ($Dy_{1.85}Fe_{17.30}$ composition) and a disordered variant of the hexagonal Th_2Ni_{17} -type structure (structure type $Y_2Fe_{17.3}$, space group $P6_3/mmc$, $Z = 2$ [8]). In this structure, a Fe dumbbell site (4e) has appeared around the (2b) Dy site, whereas an additional Dy site (2c) centers the (4f) Fe dumbbell. At the same time the (12j) Fe site was found to be split into two sites.

The R₂Fe₁₇ compounds absorb a considerable amount of hydrogen, forming stable hydrides R₂Fe₁₇H_x [7,9,10] that preserve the structure of the parent intermetallic. Hydrogen is accommodated in octahedral and tetrahedral voids preferably formed by rare-earths. Isnard *et al.* [10] investigated several R₂Fe₁₇D_x compounds by neutron diffraction and found that the octahedral hole site (6*h*) is favored for the hydrides (deuterides). Substantial occupation of the tetrahedral hole site (12*i*) occurs only for higher H concentrations ($x > 3$). A very interesting comparison can be made with the similar ternary carbides R₂Fe₁₇C_x with hexagonal Th₂Ni₁₇-type structures [11], in which carbon is accommodated in the same sites as hydrogen in the R₂Fe₁₇H_x compounds. A refinement of the structure of Dy₂Fe₁₇C_{0.5} from neutron diffraction data [12] showed that the C atoms occupy the (6*h*) interstitial site in the Th₂Ni₁₇ hexagonal structure. Haije *et al.* [13] reported that the crystal structure of Dy₂Fe₁₇C_x changes with increasing x from hexagonal (Th₂Ni₁₇-type) to rhombohedral (Th₂Zn₁₇-type).

The Dy₂Co₁₇ compound crystallizes in two polymorphic forms, a high-temperature phase with Th₂Ni₁₇-type structure and a low-temperature phase with Th₂Zn₁₇-type structure [5]. In annealed samples the Th₂Ni₁₇-type was observed as a secondary phase together with the Th₂Zn₁₇-type. When the annealing temperature was reduced, for example from 1000°C to

750°C, a remarkable increase of the fraction of the rhombohedral Th₂Zn₁₇-type was observed [3]. A single-phase Dy₂Co₁₇ sample of the Th₂Ni₁₇ type was obtained by rapid quenching of the sample in water [3]. We obtained a Dy₂Co₁₇ single crystal isotypic with Th₂Ni₁₇ from an alloy quenched after annealing at 800°C [14] (see Table 1).

The Dy₂Ni₁₇ compound only occurs in the hexagonal Th₂Ni₁₇-type structure [3].

Contrasting with the situation for R₂Fe₁₇ compounds, experimental and theoretical works on R₂Co₁₇ and R₂Ni₁₇ hydrides and carbides are very few. Only for R₂M₁₇ (R = Y, Ce, Sm; M = Co, Ni) [15] and R₂Co₁₇ (R = Pr, Sm) [16,17], hydrides with the Th₂Zn₁₇-type structure have been reported. Hydrides and carbides of the Dy₂M₁₇ (M = Co, Ni) compounds have not yet been investigated.

We found the Dy₂M₁₇ (M = Fe, Co, Ni) intermetallics and isostructural Dy₂M₁₇C_x carbides during a systematic investigation of the Dy–{Fe, Co, Ni}–C ternary systems at 800°C. In this work we carried out X-ray single crystal diffraction of Dy₂M₁₇ (M = Fe, Co, Ni) binary compounds, and explored the solubility of carbon in them. The hydrogenation capacity of the Dy₂M₁₇ and Dy₂M₁₇C_x alloys and the crystal structures of the synthesized hydrides, carbides and carbohydrides were investigated too.

Table 1 Crystal data and structure refinement parameters for Dy₂M₁₇ (M = Fe, Co, Ni).

Empirical formula	Dy _{1.79(3)} Fe _{16.84(1)}	Dy _{1.73(3)} Co ₁₇ [14]	Dy ₂ Ni ₁₇
Space group		<i>P</i> 6 ₃ / <i>mmc</i>	
<i>Z</i>		2	
Lattice parameters			
<i>a</i> , Å	8.330(2)	8.307	8.332(1)
<i>c</i> , Å	8.065(2)	8.045	8.069(1)
Unit cell volume: <i>V</i> , Å ³	484.6(1)	480.8	485.1(1)
Calculated density, g·cm ⁻³	8.734	9.165	9.057
Absorption coefficient, mm ⁻¹	39.672		47.199
Crystal size, mm ³	0.15×0.12×0.08		0.16×0.11×0.09
Radiation and wavelength, nm		Mo <i>K</i> α, 0.071073	
Diffractometer		STOE IPDS II	
Refined parameters	24		25
Refinement			
2θ _{max} and (sinθ/λ) _{max}	52.64; 0.624		58.29; 0.685
<i>h</i> , <i>k</i> , <i>l</i>	-10 ≤ <i>h</i> ≤ 9 -10 ≤ <i>k</i> ≤ 10 -10 ≤ <i>l</i> ≤ 10		-11 ≤ <i>h</i> ≤ 11 -11 ≤ <i>k</i> ≤ 11 -11 ≤ <i>l</i> ≤ 10
Collected reflections	2306		3371
Independent reflections	200 (<i>R</i> _{int} = 0.084)		260 (<i>R</i> _{int} = 0.092)
Reflections with <i>I</i> ₀ ≥ 2σ(<i>I</i> ₀)	163 (<i>R</i> _σ = 0.023)		191 (<i>R</i> _σ = 0.026)
Final <i>R</i> ₁ indices (<i>R</i> ₁ all data)	0.050 (0.08)		0.057 (0.12)
Weighted <i>wR</i> ₂ factor (<i>wR</i> ₂ all data)	0.061 (0.068)		0.071 (0.085)
Goodness-of-fit on <i>F</i> ²	1.188		1.103
Δρ _{max} and Δρ _{min} , e·Å ⁻³	+4.16; -1.53		+2.33; -2.16

Experimental details

Powders of the initial elements of high purity (not less than 99.99 wt.%) were pressed into tablets and arc-melted under Ar. The alloys were homogenized in evacuated quartz ampoules at 800°C in a muffle furnace for 30 days. After the heat treatment the ampoules with the samples were quenched in cold water.

Phase analysis of the samples was carried out using X-ray diffraction powder data obtained with a DRON-2.0 (Fe $K\alpha$) diffractometer. The STOE WinXPOW [18] program package was used. Single crystals were isolated from crushed samples after the thermal treatment. The single crystals were first examined by the Buerger precession technique, in order to establish their suitability for the subsequent data collection. The single crystal diffraction data of Dy_2M_{17} ($M = Fe, Co, Ni$) were collected at room temperature on a STOE IPDS II image plate diffractometer with monochromated Mo $K\alpha$ radiation. The starting atomic parameters were taken from the ordered Th_2Ni_{17} -type structure [2] and subsequently refined with the program SHELX-97 [19] in the WinGX program package [20] (full-matrix least-squares refinement on F^2) with anisotropic atomic displacements. The crystal structures of the Dy_2M_{17} ($M = Fe, Co, Ni$) compounds were also confirmed by the X-ray powder diffraction method, using the WinCSD software package [21].

Metallographic, quantitative and qualitative composition analyses of polished samples and single crystals were performed by energy-dispersive X-ray spectroscopy (EDXS) with a scanning electron microscope REMMA-102-2. Only the dysprosium, iron, nickel, and cobalt contents were investigated.

The hydrides were synthesized under 5 MPa hydrogen pressure, by exposure to hydrogenation at 400°C for 3 h after preliminary activation of the samples in vacuum at 550°C for 30 min. The amount of absorbed hydrogen was determined volumetrically.

Results and discussion

The crystal structure of the Dy_2M_{17} ($M = Fe, Co, Ni$) compounds was investigated on X-ray single crystal and powder diffraction data, and the structures of the carbides and hydrides were studied by the X-ray powder diffraction method. Fig. 1 shows the evolution of the X-ray diffraction patterns from the Dy_2Ni_{17} binary parent compound to Dy_2Ni_{17} carbide, hydride and carbohydride.

The crystal structure of the Dy_2Ni_{17} compound was investigated for the first time from single crystal X-ray diffraction data. Results of structural studies of Dy_2Fe_{17} and Dy_2Co_{17} single crystals have been reported earlier [7,14]. The crystal structure analysis of the Dy_2M_{17} ($M = Fe, Co, Ni$) compounds was carried out starting from the atomic positions of

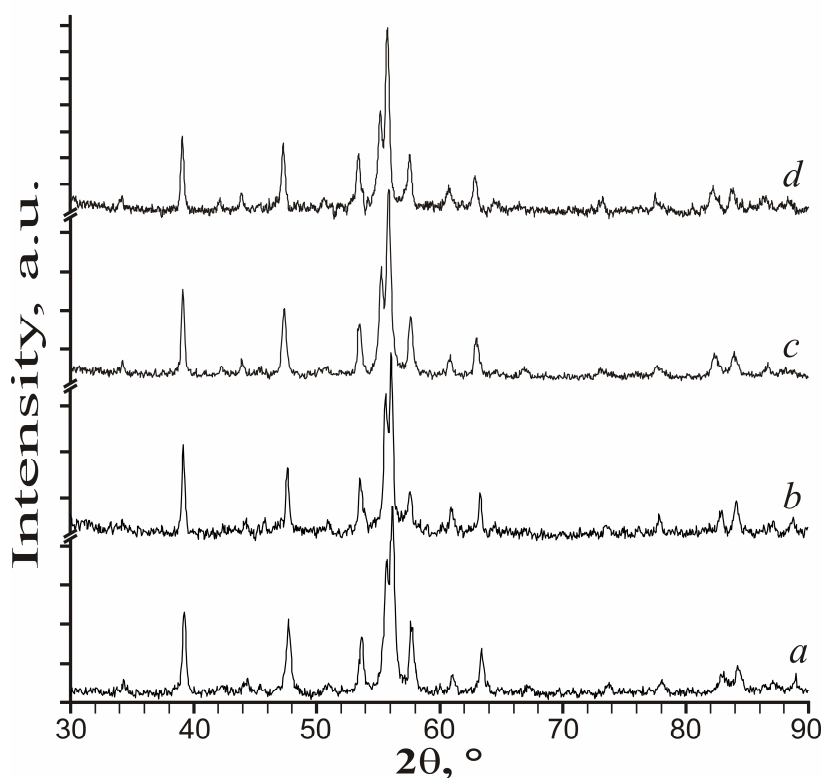


Fig. 1 X-ray diffraction profiles of the Dy_2Ni_{17} binary parent compound (a) and its carbide (b), hydride (c) and carbohydride (d).

the ordered Th₂Ni₁₇ type [2], taking into account the possibility of a disordered variant, as previously observed for Y₂Fe_{17.3} [7,8]. The crystal structure refinement showed that the Dy₂M₁₇ (*M* = Fe, Co, Ni) compounds crystallize in the Th₂Ni₁₇ structure type. Relevant crystallographic data for the Dy₂M₁₇ (*M* = Fe, Co, Ni) compounds are listed in Table 1. The atomic coordinates and thermal displacement parameters for Dy₂M₁₇ (*M* = Fe, Co, Ni) are presented in Table 2. The crystal structure investigations revealed that only the Dy₂Ni₁₇ compound had the ideal *R*:*M* stoichiometry. A small deviation from 2:17 stoichiometry was observed for both Dy₂Fe₁₇ and Dy₂Co₁₇.

Single crystals of the Dy₂Fe₁₇ compound were obtained from alloys annealed at 800°C. The refinement of the crystal structure of Dy₂Fe₁₇ showed partial occupancy of the (2*b*), (2*c*), and (4*f*) sites by Dy1, Dy2, and Fe1 atoms, respectively (see Table 2), which led to the composition Dy_{1.79(3)}Fe_{16.84(1)}. The results of the structure refinement reported in [7] led to the composition Dy_{1.85}Fe_{17.30}, which can be explained by different conditions of synthesis. The authors of [7] extracted their Dy₂Fe₁₇ single crystals from solidified polycrystalline ingots prepared by induction melting and remelting in an electric resistance furnace with a large temperature gradient and slow cooling from the melting point. It can be assumed that some differences between the crystal structure obtained in [7] and ours indicate that the Dy₂Fe₁₇ compound has a small homogeneity range leading to splitting of the (2*b*) and (4*f*) sites into (2*b*) + (4*e*) and (4*f*) + (2*c*).

During the refinement of the crystal structure of Dy₂Co₁₇ high values of the displacement parameters

of the Dy atoms were observed. The refinement of the occupancies of sites Dy1 and Dy2 led to 83(3) and 90(3) %, respectively, giving the composition Dy_{1.73(3)}Co₁₇ [14]. Thus, the result of the refinement is somewhat different from *R*_{1.89}Co₁₇, reported by Khan [5] for the isotypic compound Er₂Co₁₇.

Contrary to Er_{1.89}Co₁₇, in the structure of Dy_{1.73(3)}Co₁₇ the (2*d*), (4*f*), (12*k*) and (12*j*) sites are unfilled. The authors of [17] report an ordered model for the crystal structures of *R*₂Co₁₇ belonging to the Th₂Ni₁₇ type of structure [2]. Differently from these data, in the investigated structure of Dy_{1.73(3)}Co₁₇ the positions of the Dy atoms are not fully occupied [14].

Our systematic investigation of the Dy–{Fe, Co, Ni}–C ternary systems at 800°C showed low solubility of carbon in the Dy₂M₁₇ (*M* = Fe, Co, Ni) binary compounds, leading to the composition Dy₂M₁₇C_{*x*} (*x* < 0.5): *x* = 0.5 (*M* = Fe) [12], *x* = 0.2 (*M* = Co) and *x* = 0.4 (*M* = Ni). The Dy₂M₁₇C_{*x*} carbides preserve the Th₂Ni₁₇-type structure (see Fig. 1). The crystal structure of Dy₂Fe₁₇C_{0.5} has been investigated by neutron powder diffraction [12]. This allowed refining the crystallographic coordinates of all the atoms, including carbon. It is impossible to refine the positions of the carbon atoms from X-ray diffraction data for samples with small carbon content. However, it can be assumed that, similarly to Dy₂Fe₁₇C_{0.5}, the C atoms in the isostructural Dy₂M₁₇C_{*x*} carbides also occupy the octahedral site (6*h*: *x* 2*x* ¼, *x* ~ 0.833) in the Th₂Ni₁₇-type structure. The unit cell of the Dy₂Ni₁₇ parent compound is presented in Fig. 2. The octahedral (6*h* position) and tetrahedral (12*i* position) voids preferred by the small C and H atoms are indicated.

Table 2 Atomic coordinates and displacement parameters for Dy₂M₁₇ (*M* = Fe^a, Co^b [14], Ni^c).

Atom	Site	Occupation	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq} , Å ²
Dy1	2 <i>b</i>	0.89(2) ^a	0	0	¼	0.007(1) ^a
		0.83 ^b				0.008 ^b
		1.0 ^c				0.009(2) ^c
Dy2	2 <i>d</i>	0.90(1) ^a	⅓	⅔	¾	0.008(1) ^a
		0.90 ^b				0.010 ^b
		1.0 ^c				0.009(1) ^c
<i>M</i> 1	4 <i>f</i>	0.92(1) ^a	⅓	⅔	0.1026(2) ^a	0.011(2) ^a
		1.0 ^{b,c}				0.018 ^b
						0.016(2) ^c
<i>M</i> 2	6 <i>g</i>	1.0	½	0	0	0.010(1) ^a
						0.012 ^b
						0.013(1) ^c
<i>M</i> 3	12 <i>j</i>	1.0	0.3286(3) ^a	0.9594(2) ^a	¼	0.011(1) ^a
			0.3279 ^b	0.9591 ^b		0.017 ^b
			0.3280(3) ^c	0.9569(7) ^c		0.018(2) ^c
<i>M</i> 4	12 <i>k</i>	1.0	0.1651(2) ^a	0.3302(4) ^a	0.9807(3) ^a	0.010(2) ^a
			0.1654 ^b	0.3309 ^b	0.9800 ^b	0.013 ^b
			0.1653(6) ^c	0.3306(12) ^c	0.9788(8) ^c	0.015(2) ^c

The investigated binary Dy_2M_{17} ($M = \text{Co}, \text{Ni}$) samples absorb 3.4 ($M = \text{Co}$) and 3.5 ($M = \text{Ni}$) at. H/f.u. under 5 MPa hydrogen pressure, preserving the crystal structure of the parent compounds. The hydrogen absorption capacity of the Dy_2M_{17} ($M = \text{Co}, \text{Ni}$) alloys is close to that of the isostructural compound $\text{Ho}_2\text{Fe}_{17}$ (3.5 at. H/f.u. at 5 MPa) [10]. $\text{Dy}_2\text{Fe}_{17}$ absorbs less hydrogen, but at a lower hydrogen pressure: 3.0 at. H/f.u. at 1 MPa [7]. Hydrogenation of the Dy_2M_{17} compounds causes small changes of the interatomic distances and increases the unit cell volume (Table 3). The positional parameters of the hydrogen atoms were not refined. Taking into account the data from the neutron diffraction investigation of the crystal structure of $\text{Ho}_2\text{Fe}_{17}\text{D}_{3.6}$ [10], it can be assumed that the hydrogen atoms in $\text{Dy}_2\text{M}_{17}\text{H}_x$ hydrides also fully occupy the octahedral hole site ($6h: x 2x \frac{1}{4}, x = 0.839$) and partially occupy the tetrahedral hole site ($12i: x 0 0, x = 0.137$) in the $\text{Th}_2\text{Ni}_{17}$ -type structure (Fig. 2).

The synthesized carbides $\text{Dy}_2\text{Co}_{17}\text{C}_{0.2}$ and $\text{Dy}_2\text{Ni}_{17}\text{C}_{0.4}$ absorb 2.7 and 2.8 at. H/f.u., respectively. The obtained carbohydrides occur in the same hexagonal $\text{Th}_2\text{Ni}_{17}$ -type structure. Their lattice parameters are given in Table 3. The lattice expansion upon carbohydrogenation is anisotropic. The expansion in the basal a - b plane is larger than along the c -axis, indicating stronger interaction between the layers of metal atoms along the c -axis.

A comparison with the crystal structure of the isostructural $\text{R}_2\text{Fe}_{17}\text{C}_x$ from neutron diffraction data

[11] and $\text{R}_2\text{Fe}_{17}\text{D}_x$ [10] shows that the octahedral hole site ($6h: x 2x \frac{1}{4}, x \sim 0.833$) is favored by the carbon and deuterium (hydrogen) atoms in the carbides and deuterides (hydrides). Substantial occupation of the tetrahedral hole sites ($12i: x 0 0, x \sim 0.14$) only occurs for higher C and D(H) concentrations: $x > 3$ at. H(C)/f.u. The carbon and hydrogen atoms probably occupy the same sites ($6h: x 2x \frac{1}{4}, x \sim 0.833$) in the hexagonal $\text{Th}_2\text{Ni}_{17}$ -type structure. The addition of carbon to the binary Dy_2M_{17} alloys decreased the hydrogen capacity (see Table 3) under the same hydrogenation conditions.

Conclusions

1. X-ray single-crystal diffraction of the Dy_2M_{17} ($M = \text{Fe}, \text{Co}, \text{Ni}$) binary compounds confirmed their crystallization in the $\text{Th}_2\text{Ni}_{17}$ -type structure (space group $P6_3/mmc$).
2. The compounds exhibit low solubility of carbon: 0.2 ($M = \text{Co}$) and 0.4 ($M = \text{Ni}$) at. C/f.u. The octahedral holes ($6h: x 2x \frac{1}{4}, x \sim 0.833$) in the crystal structures are occupied by carbon atoms in $\text{Dy}_2\text{M}_{17}\text{C}_x$ ($M = \text{Co}, \text{Ni}$).
3. The hydrides $\text{Dy}_2\text{Co}_{17}\text{H}_{3.4}$, $\text{Dy}_2\text{Ni}_{17}\text{H}_{3.5}$, $\text{Dy}_2\text{Co}_{17}\text{C}_{0.2}\text{H}_{2.8}$ and $\text{Dy}_2\text{Ni}_{17}\text{C}_{0.4}\text{H}_{2.7}$ were obtained under 5 MPa hydrogen pressure after preliminary activation of the parent binary samples at 550°C for 30 min.

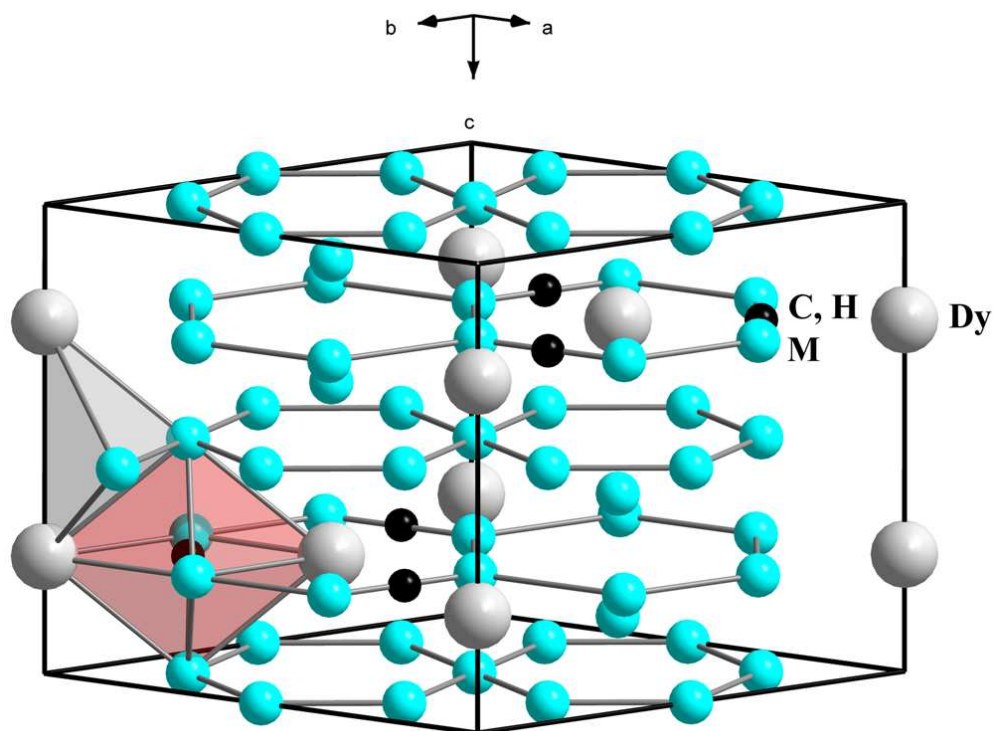


Fig. 2 Unit cell of ideal Dy_2M_{17} ($M = \text{Co}, \text{Ni}$) with $\text{Th}_2\text{Ni}_{17}$ -type structure. The octahedral ($6h: x 2x \frac{1}{4}, x \sim 0.833$) and tetrahedral ($12i: x 0 0, x \sim 0.14$) hole sites preferred by C and H atoms are indicated.

Table 3 Unit cell parameters (from X-ray powder diffraction data) and their changes (Δ) for the Dy₂M₁₇ ($M = \text{Fe}, \text{Co}, \text{Ni}$) parent compounds and their carbides, hydrides and carbohydrides.

Compound	$a, \text{\AA}$	$c, \text{\AA}$	$V, \text{\AA}^3$	$\Delta a/a_0$ (%)	$\Delta c/c_0$ (%)	$\Delta V/V_0$ (%)	Ref.
Dy ₂ Fe ₁₇	8.460	8.325	516.0				[12]
Dy ₂ Fe ₁₇ C _{0.5}	8.490	8.329	519.9	0.35	0.05	0.76	[12]
Dy ₂ Fe ₁₇ H ₃	8.546	8.343	527.7			2.27	[7]
Dy ₂ Co ₁₇	8.328	8.125	488.0				[3]
	8.330(1)	8.149(1)	489.6(2)				a
Dy ₂ Co ₁₇ C _{0.2}	8.339(1)	8.147(2)	490.7(3)	0.11	0.02	0.22	a
Dy ₂ Co ₁₇ H _{3.4}	8.3966(6)	8.1604(2)	498.3(1)	0.80	0.14	1.78	a
Dy ₂ Co ₁₇ C _{0.2} H _{2.8}	8.418(2)	8.165(2)	501.1(2)	1.06	0.20	2.34	a
Dy ₂ Ni ₁₇	8.299	8.037	479.4				[3]
	8.302(1)	8.034(2)	479.5(2)				a
Dy ₂ Ni ₁₇ C _{0.4}	8.317(4)	8.052(3)	482.3(6)	0.18	0.22	0.58	a
Dy ₂ Ni ₁₇ H _{3.5}	8.371(1)	8.049(1)	488.5(2)	0.83	0.19	1.90	a
Dy ₂ Ni ₁₇ C _{0.4} H _{2.7}	8.3789(8)	8.054(1)	489.7(2)	0.93	0.25	2.13	a

^a present investigation

4. Dy₂M₁₇C_x carbides exhibit lower hydrogen sorption capacity than the parent binaries Dy₂M₁₇. This is probably the result of C(H) occupation of the same octahedral voids in the hexagonal Th₂Ni₁₇-type structure (site 6h: $x \ 2x \ 1/4$, $x \sim 0.833$) for (C+H) concentrations ≤ 3 at./f.u. For (C+H) or H concentrations > 3 at./f.u. part of the tetrahedral voids (site 12i: $x \ 0 \ 0$, $x \sim 0.14$) are occupied by H atoms too.

All of the synthesized carbides, hydrides and carbohydrides preserve the structure of the parent binary Dy₂M₁₇ compounds. The lattice expansion during inclusion of C and/or H atoms is anisotropic. It is larger in the basal a - b plane than along the c -axis.

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