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Novel intermetallic hydrides

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Abstract

The paper focuses on structural chemistry of novel intermetallic hydrides with unusual structural properties. In such "anisotropic" hydrides, a huge expansion proceeds in a sole crystallographic direction and leads to a dramatic differentiation of the properties of the hydrides along the direction of the expansion and normal to it. The behaviour of the "anisotropic" hydrides is dominated by the metal–hydrogen and hydrogen–hydrogen interactions in contrast to the "conventional" intermetallic hydrides where the metal–metal interactions are the most important ones. In sharp contrast to the known crystal structures of intermetallic hydrides, in "anisotropic" hydrides deuterium atoms do not fill *initially existing* interstices but, instead, attract rare earth atoms into their surrounding and form *new D-occupied sites*. This paper will summarise our recent research on the "anisotropic" hydrides with a particular focus on two groups of materials: (a) RENiIn-based deuterides (RE = rare earth metal) containing the shortest known separation of hydrogen atoms in the structures of metal hydrides and (b) $RENi_3$–($CeNi_3$) and RE_2Ni_7–(La_2Ni_7)-based deuterides which develop unusually large (59–63%) expansion of the constituent $RENi_2$ layers.

Keywords: Hydrogen storage materials; Intermetallics; Neutron diffraction; Crystal structure and symmetry

1. Introduction

Hydrogenation of intermetallic compounds (IMC), from gas or electrochemically, leads to a storage of atomic, interstitial hydrogen in the metal lattice providing a high ratio of H/M (>1) and a high volume density of the stored hydrogen compared to liquid hydrogen. Intermetallic hydrides exhibit a close interrelation between crystal chemistry and hydrogen sorption properties allowing alteration and optimisation of their H storage performance. Hydrogen accommodation by the metal lattice is typically accompanied by modest (few percent) changes of the interatomic metal–metal distances. Consequently, H atoms enter the interstices, which are originally available in the virgin intermetallics. However, this "typical" case does not cover a large group of very interesting and so far insufficiently studied compounds, the so-called "anisotropic" hydrides. In such hydrides, a huge expansion proceeds in a sole crystallographic direction and leads to a dramatic differentiation of the properties of the hydrides along the direction of the expansion and normal to it. This paper will summarise our recent research on the "anisotropic" hydrides with a particular focus on two groups of materials.

(a) RENiIn-based deuterides (RE = rare earth metal) containing the shortest known separation of hydrogen atoms in the structures of metal hydrides, 1.56–1.60 Å and, consequently, providing the highest local volume content of H [1]. The effect of substitution of the constituent elements, RE, Ni and In, on the crystal structure and thermodynamics of the IMC–H_2 systems, will be presented and discussed.
(b) $RENi_3$–($CeNi_3$) and RE_2Ni_7–(La_2Ni_7)-based deuterides are built from the two kinds of metal slabs, $RENi_5$ and $RENi_2$. They stack along $[0\,0\,1]_{hex}$, the direction of anisotropic expansion of the lattice. Such an expansion (20–31%) proceeds within the $RENi_2$ slabs only and leads to an incredible (59–63%) expansion of these layers. In sharp contrast to the known crystal structures of intermetallic hydrides, in $CeNi_3D_{2.8}$ [2] and $La_2Ni_7D_{6.5}$

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(present study) deuterium atoms do not fill *initially existing* interstices but, instead, attract rare earth atoms into their surrounding and form *new D-occupied sites*, RE_3Ni and RE_3Ni_3.

The behaviour of the “anisotropic” hydrides is dominated by the metal–hydrogen and hydrogen–hydrogen interactions in contrast to the “conventional” intermetallic hydrides where the metal–metal interactions are the most important ones.

2. Experimental

The alloys were prepared by arc melting of mixtures of high purity constituent metals. A slight excess of rare earth metals, 1 at.%, was used to compensate their evaporation during the melting. As cast alloys were sealed into the evacuated quartz tubes and homogenised by high-temperature annealing, followed by quenching into the mixture of ice and water.

Phase-structural composition of the alloy and their corresponding hydrides was characterised by powder X-ray diffraction (Siemens D5000 diffractometer; Cu $K\alpha_1$ radiation; Bragg–Brentano geometry; position sensitive detector).

The prepared alloys were first activated by heating for 1 h at 400 °C in secondary vacuum ($\sim 10^{-5}$ mbar) and then saturated with deuterium gas (99.8% purity) under pressures of 1–10 bar D_2.

The deuterides were studied either ex situ (in *V* cans filled by Ar) or in situ under the pressure of deuterium gas. In the latter case, they were placed into the quartz tube ($CeNi_3D_{2.8}$) or into the stainless steel autoclave ($NdNi_{1-x}Cu_xIn_{1-y}Al_yD_z$).

Powder neutron diffraction (PND) data were collected at the R2 reactor at Studsvik Neutron Research Laboratory using SLAD instrument ($\lambda = 1.117$ Å) and the high-resolution diffractometer NPD ($\lambda = 1.470$ Å). The NPD instrument uses 35 ^{3}He counters to measure the intensities in 2θ steps of 0.08° to cover a 2θ range of 4.0–137°. The SLAD instrument uses a position sensitive detector system. The data were fully corrected for scattering due to the absorption and then normalised to the vanadium standard. During the refinements of the in situ experiments peaks from the stainless steel tube were excluded from the refinements.

The PND studies of the $CeNi_3D_{2.8}$ were performed on the D1B diffractometer, Institute Laue Langevin, Grenoble.

Crystal structure data were derived by Rietveld profile refinements using the GSAS software [3].

3. RENiIn-based hydrides

NdNiIn intermetallic crystallises with the ZrNiAl-type hexagonal structure (space group $P\bar{6}2m$; $a = 7.5202$; $c = 3.9278$ Å). Two different deuterides, β (0.4–0.67 at.H/f.u.) and γ (1.2–1.6 at.H/f.u.) formed by NdNiIn were structurally characterised by PND [1]. Structural properties of the higher, γ-deuteride $NdNiInD_{1.2}$ are very unusual. It is formed via anisotropic expansion of the hexagonal unit cell along [0 0 1] ($\Delta c/c = 16.5\%$) leading to the *double* occupancy of the trigonal bypiramidal (TB) sites Nd_3Ni1_2 and a formation of the D···D pairs with D–D distance of 1.56 Å (Fig. 1). At lower D content, in the β-deuteride $NdNiInD_{0.6}$, half of hydrogen is removed from the bypiramidal sites and deuterium atoms randomly occupy every second Nd_3Ni1 tetrahedron. Volume expansion in this case is relatively small, 3.6%, and isotropic.

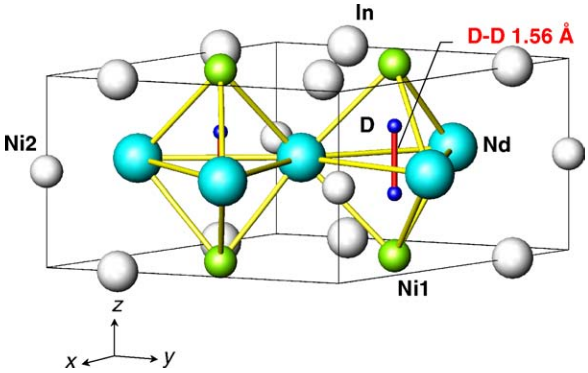


Fig. 1. Crystal structure of $NdNiInD_{1.2}$ containing short D–D distances of 1.56 Å. 3 Nd in 3*g* (0.6440, 0, 1/2); 2 Ni1 in 2*c* (1/3, 2/3, 0); 1 Ni2 in 1*b* (0, 0, 1/2); 3 In in 3*f* (0.2473, 0, 0); 3.6 D in 4*h* (1/3, 2/3, 0.6707).

The most important feature of the $NdNiInD_{1.2}$ is that it does not obey the “rule of 2 Å”, empirically known for the metal hydrides, the shortest found separation between hydrogen atoms which has been considered as a lowest possible value for the distance between H atoms thus imposing limits on the maximum volume hydrogen storage capacity of the metal hydrides. Naturally, a decrease in this limiting distance down from 2 Å leads to a corresponding rise in the volume content of hydrogen in the metal hydrides.

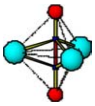
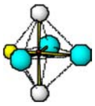
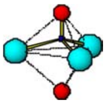
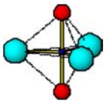
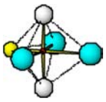
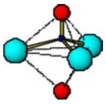
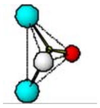
In order to understand better the reasons for the H···H pairing in the NdNiIn-based hydrides, we have studied the effect of the replacement of the constituent elements by chemically related substitutes on the structural and thermodynamic behaviours. Ni substitution by Cu and In substitution by Al have been tried. Two related to NdNiIn equiatomic ABC intermetallics, NdCuIn ($a = 7.480$; $c = 4.219$ Å) and NdNiAl ($a = 7.016$; $c = 4.062$ Å) are isostructural to NdNiIn and crystallise with the ZrNiAl type structures. Opposite volume effects are observed on substitution: unit cell volume for the Cu compound is 6.2% higher compared to NdNiIn, while Al-based intermetallic has a significantly contracted unit cell ($\Delta V/V = -10\%$).

A complete range of solid solutions is formed between NdNiIn and NdCuIn; a gradual increase of c_{hex} and *V* accompanies an increase of Cu content. In contrast, in case of Al, only a limited solubility takes place between compositions NdNiIn and $NdNiIn_{0.75}Al_{0.25}$. The substitution significantly decreases both *a* and *V* leaving *c* practically constant. Three types of interstices most favourable for the insertion of hydrogen atoms, which exist in the structures of the Nd(Ni,Cu)(In,Al) intermetallic alloys are shown in Fig. 2: TB

Table 1
Ni/Cu distribution in the 2*c* and 1*b* sites of the $NdNi_{1-x}Cu_xIn$-based materials

	Ni/Cu stoichiometry	Ni/Cu 2*c* (PND)	Ni/Cu 1*b* (PND)	$d_{Ni(Cu)–D}$ (Å, PND)
$NdNi_{0.75}Cu_{0.25}In$	3/1	7/1	1/1	1.667
$NdNi_{0.50}Cu_{0.50}In$	1/1	7/4	1/3	1.84

Table 2
Types of hydrides formed in the $NdNi_{1-x}Cu_xIn_{1-y}Al_y–D_2$ systems

	Structure type of hydride	*x*	*y*	Expansion	Filled interstices (as in Fig. 2)	
I	γ-$LaNiInD_{1.63}$ [3]	≤0.05	≤0.05	A		
II	β-$RNiInD_{0.67}$ [1]	≥0.25	0	I		
III	$NdNiIn_{0.875}Al_{0.125}D_{0.7}$	0	0.125	I		
IV	$NdNiIn_{0.75}Al_{0.25}D_{1.3}$	0	0.25	A		

A, anisotropic; I, isotropic.

Type II hydrides are present as secondary phases in all the Type I hydrides-based samples. (I) D–D pair in Nd_3Ni1_2 (D1) + D in Nd_3Ni2In_2 (D2); (II) single occupancy of the Nd_3Ni1; (III) single occupancy of the Nd_3Ni1 (D1) + D in Nd_3Ni2In_2 (D2); (IV) single occupancy of the Nd_3Ni1 (D1) + D in Nd_2Ni1In (D2).

$Nd_3[(Ni,Cu)1]_2$; O octahedron $Nd_3[(Ni,Cu)2](In,Al)_2$ and T tetrahedron $Nd_2(In,Al)[(Ni,Cu)1]$.

Analysis of the PND data concludes that Cu substitution for Ni proceeds with a strong preference for the 1*b* site (Table 1); the level of Ni substitution in the 2*c* site is much lower. In the 1*b* site, transition element is surrounded by a trigonal prism of In. Possibly, In–Cu bonds are stronger compared to the Ni–In ones.

Substitutions significantly affect the mechanism of the formation of the hydrides. Four different types of the hydrides were identified in the studied systems and are characterised in Table 2.

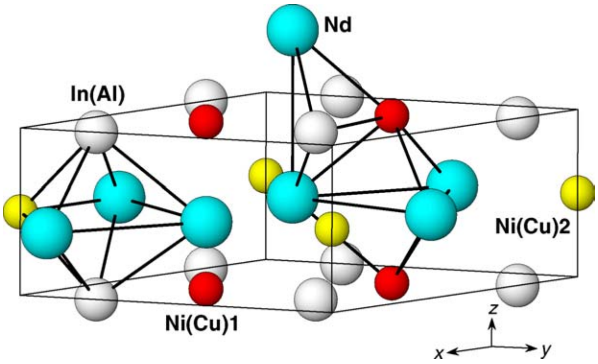


Fig. 2. Hexagonal ZrNiAl-type structure formed in the Nd(Ni,Cu)(In,Al) alloys. Three most favourable for the insertion of hydrogen atoms types of interstices, TB $Nd_3[(Ni,Cu)1]_2$, O $Nd_3[(Ni,Cu)2](In,Al)_2$ and T $Nd_2(In,Al)[(Ni,Cu)1]$ are shown.

Hydride I containing the D···D pair was formed in the samples with low copper and aluminium contents ($x \leq 0.05$) only. In addition to the double-occupied Nd_3Ni1_2 trigonal bipyramids, the octahedral $Nd_3Ni(Cu)2In_2$ sites are simultaneously filled by D atoms. It seems that the filling of these sites becomes possible only as associated with the formation of short D–D distances in the trigonal bipyramid. The probable reason for that is an isotropic expansion of the unit cell which makes In–D2 distances sufficiently large (In–D ≈2.28 Å) thus lifting the blocking effect of In on hydrogen insertion into the site.

4. $RENi_3–D_2$ and $RE_2Ni_7–D_2$ systems

From structural point of view, in $NdNiInD_{1.2}$, the appearance of short H–H distances correlates with an anisotropic uniaxial lattice expansion on hydrogenation (16%). Thus, we have extended our studies to the hydrides where this feature is even more pronounced.

One important example of “anisotropic” structures represents hexagonal (trigonal) hydrides formed on the basis of $RENi_3$ and RE_2Ni_7 intermetallics in the binary systems of rare earth metals with nickel. Their crystal structures are closely related, and can be presented as a stacking of the

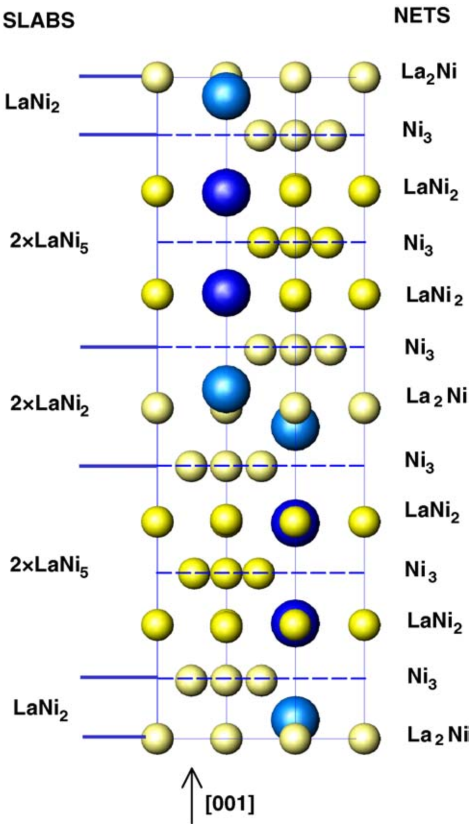


Fig. 3. The crystal structure of La_2Ni_7 shown as composed of the slabs $LaNi_2$ and $LaNi_5$ and the nets $LaNi_2$, Ni_3 and La_2Ni.

$CaCu_5$- and $MgZn_2$-type slabs along [0 0 1]. Combination $1 \times RENi_5 + 2 \times RENi_2$ provides the overall stoichiometry $3 \times RENi_3$. For the RE_2Ni_7 compounds the ratio of the $RENi_5$ and $RENi_2$ slabs is 1:1. $CeNi_3$ structure contains 12 types of tetrahedral sites with three kinds of surrounding, Ce_2Ni_2, $CeNi_3$ and Ni_4. The same type of the surrounding of the tetrahedral sites, RE_2Ni_2, $RENi_3$ and Ni_4, can be found for the RE_2Ni_7 crystal structures. Stacking of the $LaNi_2$ and $LaNi_5$ slabs and containing the plain (Ni_3 and $LaNi_2$) and "buckled" (La_2Ni) nets in the structure of La_2Ni_7 is shown in Fig. 3.

5. $CeNi_3D_{2.8}$

During the hydrogenation, the hexagonal $CeNi_3$ transforms into an orthorhombic $CeNi_3D_{2.8}$ and an extremely pronounced expansion along the [0 0 1] direction, 30.7%, occurs [2]. PND of this deuteride has shown that in the $CeNi_3D_{2.8}$ the lattice elongation does not touch the $CeNi_5$ parts which even "shrink" along [0 0 1] (−2.8%). This contrasts to the behaviour of the $CeNi_2$ slabs where the expansion is uniquely high (63.1%). Thus, the metal sublattice is completely rebuilt. Especially pronounced changes are observed for the chains of the Ni_4 and $CeNi_3$ tetrahedra, which are aligned along [0 0 1]. In the $CeNi_3$ intermetallic compound the Ni_4 tetrahedra are nearly regular. In contrast, after the expansion to form $CeNi_3D_{2.8}$ some of these tetrahedra become so expanded that they do not exist any more (see Table 3). The same conclusion is valid for the aligned along [0 0 1] $CeNi_3$ sites: Ce–Ni bonding is broken in the 0 0 z direction.

Occupancy/vacancy of the $CeNi_2$ and $CeNi_5$ parts by deuterium is in agreement with the observed values of volume expansion. All D atoms are located inside the $CeNi_2$ part and on the border of $CeNi_2$ and $CeNi_5$ leaving $CaCu_5$-type part empty. Deuterium atoms occupy eight different sites. The limiting stoichiometric composition is $D/CeNi_3 = 3.0$.

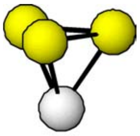
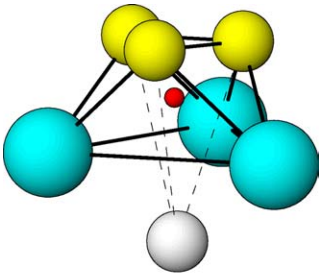
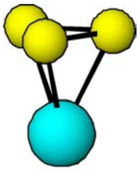
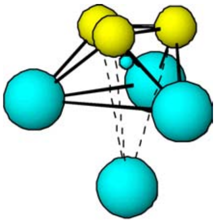
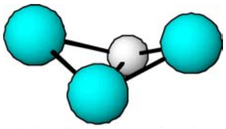
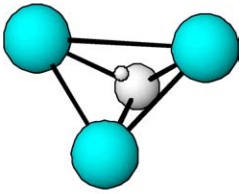
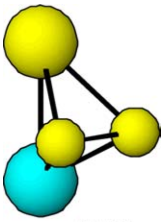
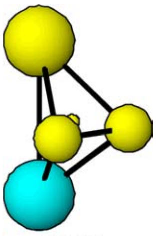
6. $La_2Ni_7D_{6.5}$

Studies of the crystallographically similar to $CeNi_3D_{2.8}$ anisotropic hydrides are necessary to understand general features governing their formation. A related new example is the $La_2Ni_7D_{6.5}$ deuteride. The hexagonal crystal structure of the original La_2Ni_7 intermetallic alloy (Ce_2Ni_7 type of structure; space group $P6_3/mmc$; $a = 5.059(3)$; $c = 24.68(2)$ Å) similarly to $CeNi_3$ expands exclusively along [0 0 1] ($La_2Ni_7D_{6.5}$: $a = 4.9534(6)$; $c = 29.579(5)$ Å; $\Delta a/a = -2.1\%$; $\Delta c/c = 19.8\%$; $\Delta V/V = 14.9\%$). The expansion is less pronounced compared to $CeNi_3D_{2.8}$. The observed in present study volume expansion of the unit cell of La_2Ni_7 on hydrogenation is less pronounced compared to the data published in [4] for $La_2Ni_7H_x$ ($a = 5.01$; $c = 31.0$ Å; $\Delta V/V = 23.1\%$). This difference indicates that further hydrogen absorption takes place during an increase of the synthesis pressure from 10 bar used in current work to 80 bar H_2 applied in [4].

For the two types of the constituent slabs, the hydrogenation behaviour is opposite: the $MgZn_2$-type slab expands along c by 58.7% while the $CaCu_5$-type slab remains unaffected by hydrogen absorption and even slightly shrinks ($\Delta c/c = -0.5\%$). These features of the crystal structure of $La_2Ni_7D_{6.5}$ completely resemble the behaviour of $CeNi_3D_{2.8}$.

Furthermore, PND study revealed that hydrogen does not enter the $LaNi_5$ layers at all residing only at the borders of the $LaNi_5$ and $LaNi_2$ slabs (within the Kagome Ni-nets) and inside the $LaNi_2$ slabs. In total, four different sites are filled with D. All three interstitial sites occupied by D inside the $LaNi_2$ layers do not exist in the initial crystal structures and are formed during a modification of the crystal structure of La_2Ni_7 on hydrogenation. These sites include two types of the La_3Ni_3 octahedra and one type of the La_3Ni tetrahedron. In addition, deuterium atoms fill the La_2Ni_2 tetrahedra, which are present in the original structure of La_2Ni_7 and equally belong to $LaNi_2$ and $LaNi_5$ slabs. Deuterium content of the $LaNi_2$ slabs is rather high, 5 at.D/f.u. in maximum. Approximately 1/4 of the overall deuterium content is associated with the $LaNi_5$ slab (1.5 at.D/f.u.; $La_2Ni_7D_{6.5} = LaNi_2D_{5.0} + LaNi_5D_{1.5}$). The Rietveld plot of the NPD data for $La_2Ni_7D_{6.5}$ is shown in Fig. 4. The crystal structure data for $La_2Ni_7D_{6.5}$ are given in Table 4.

Table 3
Coordination of the D atoms in the structures of $CeNi_3D_{2.8}$ and $La_2Ni_7D_{6.5}$ as related to the interstices available in the crystal structures of intermetallic compounds

Intermetallic alloy	Deuteride	$CeNi_3D_{2.8}$	$La_2Ni_7D_{6.5}$
New coordination of D is achieved via deformation of the metal sublattice			
 Ni_4	 RE_3Ni_3	D1 D6	D1
 RNi_3	 RE_3Ni_3	D2 D7	D2
Formation of a new type of interstice due to the strong expansion of the $MgZn_2$-type layer			
 Interstice does not exist	 RE_3Ni	D3 D5	D3
Filling of the available RE_2Ni_2 tetrahedra at the boundary between the $CaCu_5$- and $MgZn_2$-type layers			
 RE_2Ni_2	 RE_2Ni_2	D4 D8	D4

All D–D distances in the structure are high and exceed 1.8 Å. Maximum stoichiometric composition, which can be reached by increasing the occupancy of the 50% filled D3 site to 100%, is $La_2Ni_7D_{8.0}$. This will not require any extra deformation of the structure. The shortest Ni–D and La–D distances are 1.515(5) and 2.385(18) Å, respectively.

Further D uptake inside the $LaNi_5$ layers is anticipated at higher D_2 pressures with D entering the La_2Ni_2 sites inside the $LaNi_5$ layers and, in addition, the $LaNi_3$ (12*n* in the $LaNi_5$ structure) sites.

An ordered hydrogen sublattice in the structure of $La_2Ni_7D_{6.5}$ can be described as a stacking of the 15-vertex coordination polyhedra formed by D around the La atoms belonging to the $LaNi_2$ slabs (see Fig. 5).

Analysis shows that Ni-hydrogen interaction in $La_2Ni_7D_{6.5}$ does not result in a formation of the NiH_4 units observed for the complex Ni-containing hydrides.

The most important common features of the formation of the crystal structures of $CeNi_3D_{2.8}$ and $La_2Ni_7D_{6.5}$ related to the coordination of H atoms in their structures are summarized in Table 3. As can be seen from this table, "traditional" mechanism of hydrogenation when H atoms enter the available in the crystal lattice interstitial sites (tetrahedra RE_2Ni_2), the other occupied by D sites are formed via a pronounced

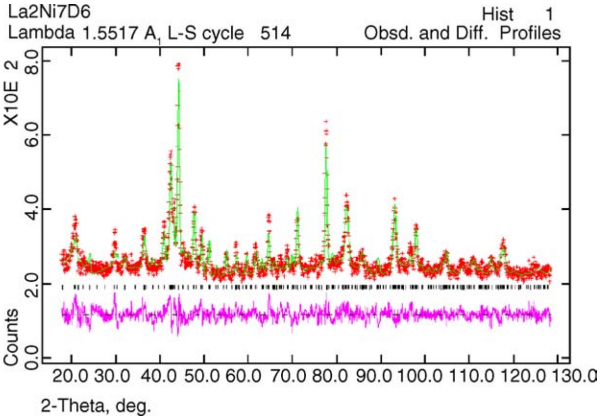


Fig. 4. Powder neutron diffraction pattern for $La_2Ni_7D_{6.5}$ (NPD instrument, $\lambda = 1.5517$ Å) showing observed (dots), calculated (line) and difference (line in bottom) pattern. Positions of the peaks are marked. $R_p = 4.41\%$; $R_{wp} = 5.57\%$.

deformation of the structures. This deformation significantly increases amount of rare earth atoms in the surrounding of H (RE_3Ni_3 octahedra) or even creates new tetrahedral sites RE_3Ni.

Comparison of the structural features of two different anisotropic hydrides, $CeNi_3D_{2.8}$ and $La_2Ni_7D_{6.5}$, allows drawing the following conclusions.

(a) Both types of the initial structures, $RENi_3$ and RE_2Ni_7, are composed of the slabs with a compositions $RENi_5$ ($CaCu_5$-type) and $RENi_2$ (Laves phase type), which stack in different sequence (1:2 and 1:1, respectively) along the *c*-axis of the hexagonal (trigonal) unit cells. At low applied hydrogenation pressures, all expansion of the "composite" unit cells proceeds within the $RENi_2$ layers only and is very anisotropic confined to the [0 0 1] direction. Within the layers with the compositions $LaNi_2$ and $CeNi_2$, the expansion is very similar being close to 60%.

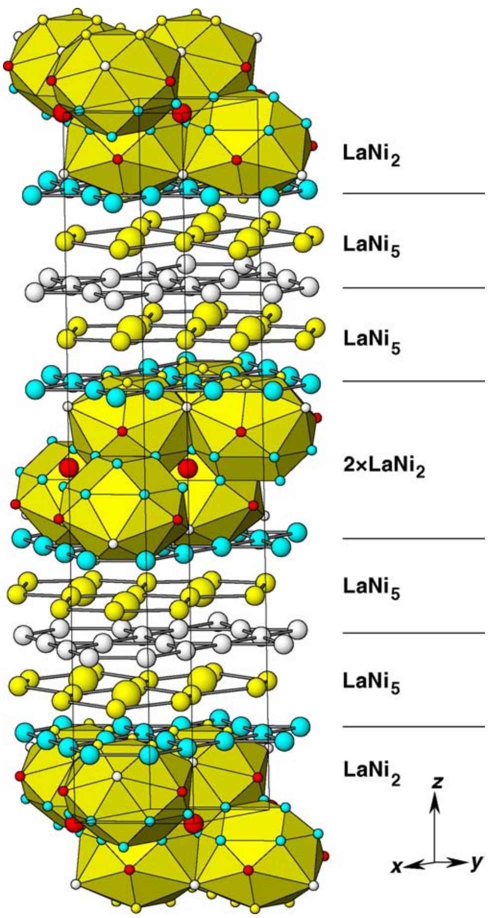


Fig. 5. Deuterium sublattice in the crystal structure of $La_2Ni_7D_{6.5}$ built as a stacking of the LaD_{15} polyhedra.

(b) The absorbed hydrogen does not enter the $RENi_5$ layers and is accumulated exclusively inside the $RENi_2$ slabs and on their borders.

(c) A deformation of the $RENi_2$ layers occupied by H is so significant that the stacking and coordination characteristics of the metal atoms in these layers are significantly

Table 4
Crystal structure data for $La_2Ni_7D_{6.5}$

Atoms	Site	*x*	*y*	*z*	Uiso ($\times 10^{-2}$ Å^2)	D surrounding
La1	4*f*	1/3	2/3	0.4514(8)	3.3(8)	
La2	4*f*	1/3	2/3	0.3124(7)	1.4(5)	
Ni1	2*a*	0	0	0	1.6(5)	
Ni2	4*e*	0	0	0.3188(8)	3.7(7)	
Ni3	4*f*	1/3	2/3	0.6854(7)	3.3(4)	
Ni4	6*h*	0.840(2)	0.679(4)	1/4	1.0(3)	
Ni5	12*k*	0.834(1)	0.668(3)	0.3868(2)	0.6(2)	
D1	4*e*	0	0	0.0864(8)	3.5	O $La1_3Ni5_3$
D2	4*f*	1/3	2/3	0.5586(11)	3.5	O $La1_3Ni5_3$
D3	12*k*	0.330(6)	0.165(3)	0.020(5)	3.5	T $La1_3Ni1$
D4	12*k*	0.485(3)	0.970(6)	0.120(1)	3.5	T $La1La2Ni5_2$

Space group $P6_3/mmc$; $a = 4.9534(6)$; $c = 29.579(5)$ Å.
Occupancy $n = 0.5$ for D3. For all other D atoms, it was constrained to $n = 1$.
Actual deuterium content in the deuteride will be refined further using the data of the PCT studies, which are in progress. The latter studies indicate (R.V. Denys, unpublished results) that it could be close to 5 at./f.u.La_2Ni_7 slightly reducing the occupancy of the completely filled D sites to approximately 77%.

modified creating new types of positions (octahedra RE_3Ni_3, tetrahedra RE_3Ni) which do not exist in the original structures and became occupied by H.

(d) The RE–H and H–H interactions dominate the structural behaviour of these anisotropic hydrides. Their hydrogen sublattices contains H atoms with all interatomic H–H separations greater then 1.8 Å, which can be built as 12-, 7- or 15-vertex polyhedra formed by D around Ce or La.

(e) Since the behaviour of La- and Ce-containing hydrides is essentially very similar, the structural features of the anisotropic hydrides do not have roots in the valence decrease of Ce during the hydrogenation.

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