

Study of hydrogenation pathway of NdScSi

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The use of hydrogen as an energy carrier for mass applications requires developing methods of effective and safe storage. Storage as hydride in intermetallic has already shown its interest from the point of view of both mass capacity and security (e.g. compounds LaNi₅ in Ni / MH batteries). Because of its high hydrogen storage capacity, magnesium and its alloys are studied by many research groups. The Mg-rich part of a RE–TM–Mg ternary diagram (RE = rare earth and TM = transition metal) is not investigated as intensively as the binary magnesium alloys but is still of great interest for several practical applications and could lead to the discovery of new interesting phases. For instance, the Mg-rich part of the Mg–Zn–RE system was studied to find new light structural materials with good corrosion resistance.

Our current research focuses on the synthesis and characterization of new intermetallic rich in magnesium. We have been studying two compounds in November 2014: NdNiMg₅ and NdScSi.

For the first one, the system is more complicated than expected and the results are still under refinement. For the second one, the aim was to study the deuteration process in NdScSi by neutron diffraction and to determine the crystal structure of the deuteride NdScSiD_x.

The *in-situ* deuteration was performed from room temperature to 400°C. Upon heating, additional nuclear peaks appear in Bragg positions slightly shifted from those of NdScSi. This corresponds to the appearance of the deuterated phase. After 26 h of heating under 5 bar of D₂ and up to 350°C the parent phase NdScSi has completely disappeared and only the peaks of the deuteride are present.

A refinement of the crystal structure was performed (figure 1), the crystal data are gathered in table 1. All peaks are indexed with the tetragonal space group I4/mmm and the NdScSi keeps its initial CeScSi-type structure upon deuteration. We observe a slight decrease of the *a* parameter from 4.2837 to 4.1872 Å and a strong increase of the *c* parameter from 15.686 to 16.628 Å.

In the structure (figure 2), the deuterium atoms completely occupy the [Nd₄] tetrahedral sites in D1 (0 0.5 0.25). Such structural behavior is similar to that observed for CeFeSi-type compounds. Additionally, D atoms also occupy [NdSc₄] square based pyramidal sites in D2 (0 0 0.518). This site is only half filled since otherwise it would induce to small interatomic distances between D2 atoms. It is noteworthy that the D2 atoms are slightly shifted from the [Sc₄] square plane towards the Nd atom. The *in-situ* deuteration study has also revealed that both sites are filled simultaneously.

Table 1. Crystal structure parameters of NdScSiD_{1.5} (RB = 3.4 %).

Atom	Site	x	y	z	Occ
Nd	4e	0	0	0.316	1
Sc	4c	0	1/2	0	1
Si	4e	0	0	0.110	1
D1	4d	0	0.5	0.25	1.01(1)
D2	4e	0	0	0.518	0.47(1)

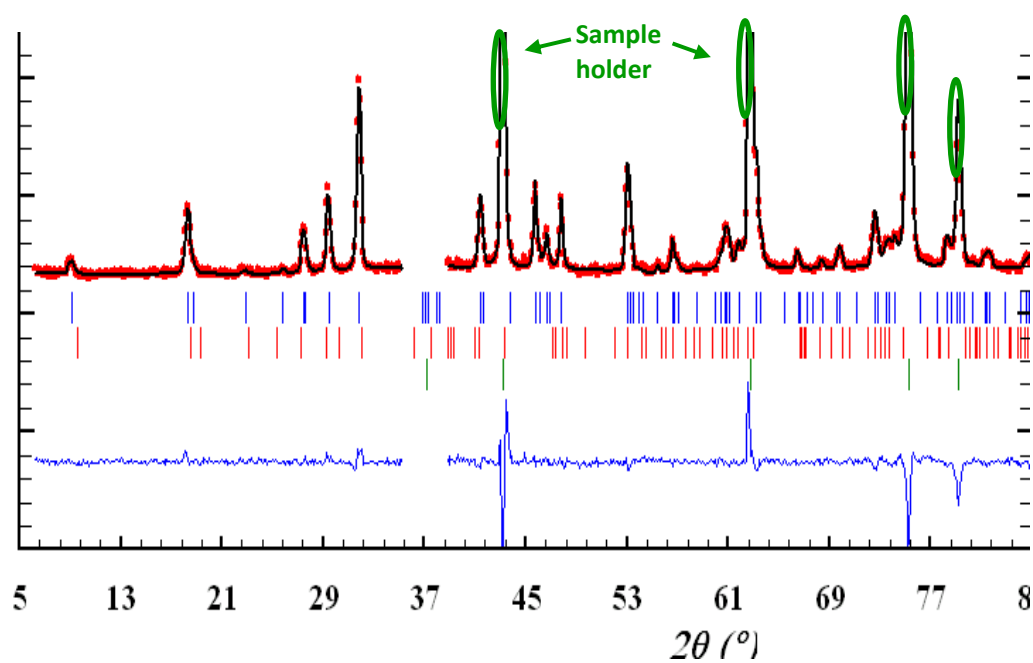


Figure 1 Neutron diffraction pattern and refinement at 300 K of $\text{NdScSi}_{1.5}$. The second line of ticks correspond to the initial Bragg position of NdScSi .

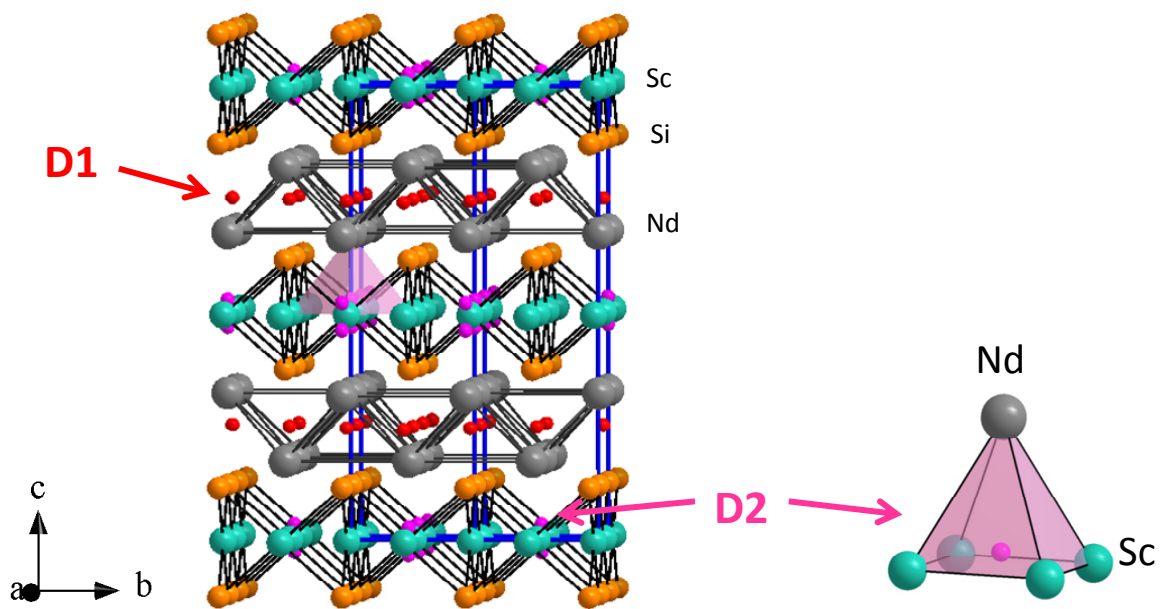


Figure 2 Crystal structure of $\text{NdScSi}_{1.5}$. A zoom of the D2 square based pyramidal site is shown on the right part.