

La₂MgNi₂H₈, the first mixed polynuclear transition metal hydride

1 - Synopsis

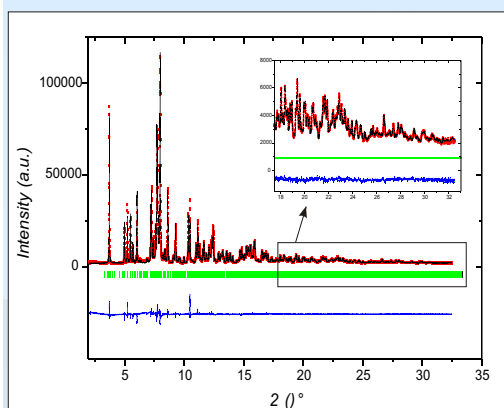
The structure of La₂Mg₂Ni₂H₈ (48 positional parameters) has been solved from synchrotron and neutron powder diffraction data. It is the first case of a complex transition metal hydride containing two types of polynuclear hydride complexes [Ni₄H₁₂]¹²⁻ and [Ni₂H₇]⁷⁻.

2 - Introduction

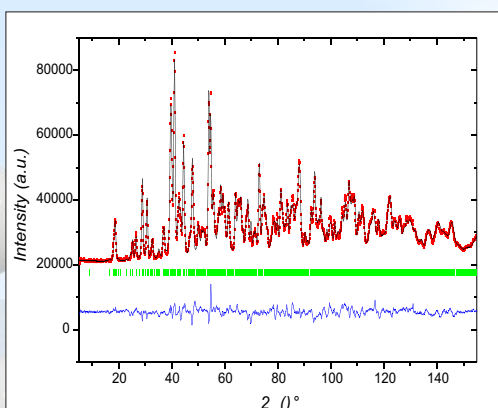
Following our recent discovery of a hydrogen-induced insulating state in the LaMg₂Ni-H system we have investigated the closely related La₂MgNi₂-H system. Hydrogenation of tetragonal La₂MgNi₂ at 10 bar and 100°C leads to a complex metal hydride of composition La₂MgNi₂H₈ having monoclinic symmetry.

3 - Synchrotron and neutron diffraction

Synchrotron and neutron data were collected at room temperature.



Synchrotron powder diffraction pattern of a deuteride sample measured at the ESRF (SNBL). $\lambda = 0.37504 \text{ \AA}$.



Neutron powder diffraction pattern of a deuteride sample measured at PSI (HRPT). $\lambda = 1.88577 \text{ \AA}$.

Crystallographic data (from synchrotron):

26 independent atoms

Space group: $P2_1/c$, $Z = 8$

$a = 11.84482(1) \text{ \AA}$

$b = 7.821099(8) \text{ \AA}$

$c = 11.96310(1) \text{ \AA}$

$\beta = 92.780(1)^\circ$

$V = 1106.96(2) \text{ \AA}^3$

Reliability factors:

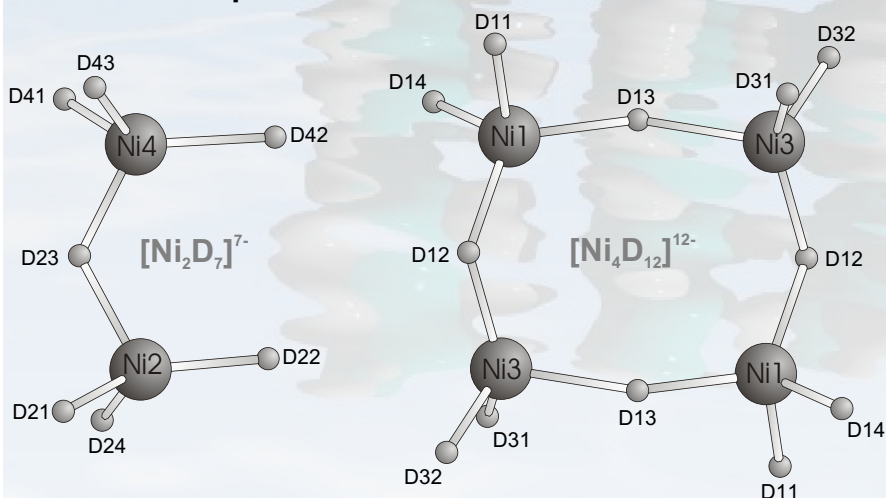
$R_p = 0.069$, $R_{wp} = 0.081$, $\chi^2 = 12.7$ (synchrotron)

$R_p = 0.078$, $R_{wp} = 0.090$, $\chi^2 = 26.9$ (neutron)

4 - Structure of the deuteride: 2 polynuclear deuterido complexes

16 independent crystallographic sites of deuterium atoms were found using FOX. Atomic positions were refined using FullProf.

13 "complexes" deuterium



3 "interstitial" deuterium

