

## STRUCTURE AND PHASE TRANSITIONS

**[C7. O.L. Makarova] Role of topology on the magneto-structural coupling in new Laves hydrides**

Intricate magnetic and structural phenomena in the Laves phases ( $\text{RMn}_2$ ) and their hydrides come from the magnetic instability (transition from localized to itinerant states) in the Mn sublattice, which is governed by the value of the first-neighbor Mn-Mn distance. On the other hand, the topological frustration in the Mn sublattice could contribute to an unusually strong magneto-structural coupling [1-5]. Recently, progress in high-pressure high-temperature synthesis offered the opportunity to study the magnetic and crystal structures of the same chemical compounds, having the same Mn-Mn distances, but different crystal structures: cubic or hexagonal. Our results show that topology plays a dominant role in the formation of the magnetic ordering (short-range or long-range) and also affects the transition from the localized to the magnetic itinerant state.

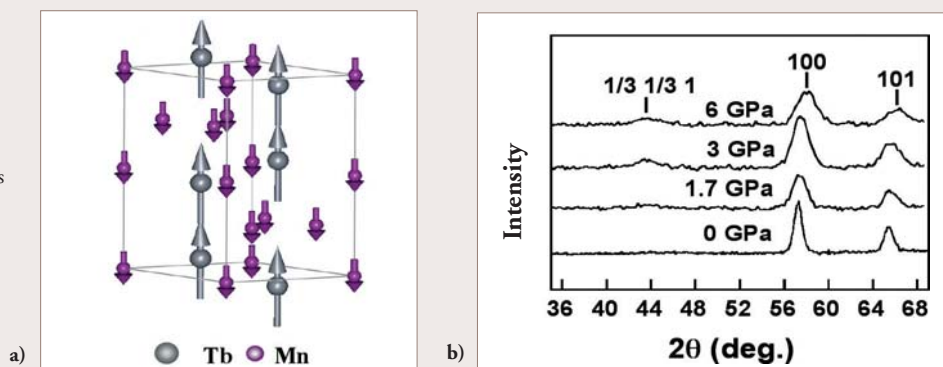
[1] I.N. Goncharenko et al Phys. Rev. B, **56**, 2580, (1997) ; [2] I.N. Goncharenko et al Phys. Rev. B, **59**, 9324, (1999)

[3] O.L. Makarova et al Phys. Rev. B, **66**, 104423, (2002) ; [4] O.L. Makarova et al Phys. Rev. B, **67**, 134418, (2003)

[5] O. L. Makarova et al Solid State Com., **132**, 329, (2004)

[Collaboration: O.L. Makarova, RRC « Kurchatov Institute », Moscow, Russia ; I.N. Goncharenko, I. Mirebeau, F. Bourée, LLB ; A.V. Tsvyaschenko, IHPP, Troitsk, Russia ; L.N. Fomicheva, IHPP, Troitsk, Russia]

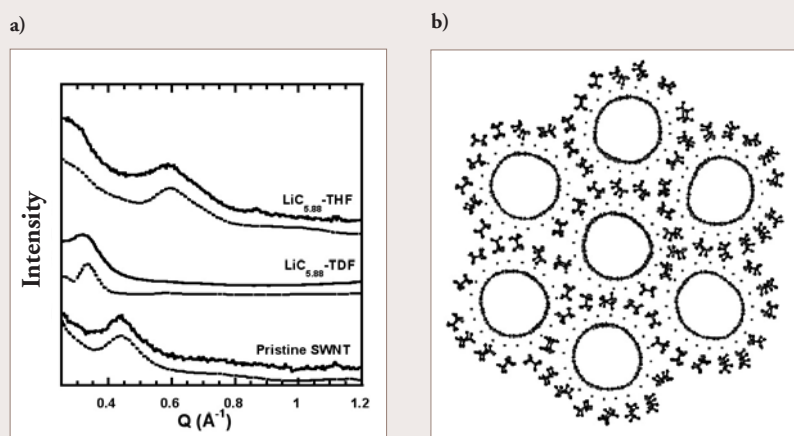
**Figure:** a) Magnetic structure of the hexagonal hydride  $\text{TbMn}_2\text{H}_{2.9}$ .  
b) Magnetic neutron diffraction spectra of  $\text{TbMn}_2\text{D}_{2.9}$  measured at different pressures and  $T=1.4\text{K}$  at the G6.1 diffractometer. The presence of the  $(1/3\ 1/3\ 1)$  reflection indicates a pressure-induced long-range antiferromagnetic component.

**[C8. J. Cambedouzou] Tunable intertube spacing in single-walled carbon nanotubes**

The structure of ternary compounds made of alkali, tetrahydrofuran (THF) and single-walled carbon nanotubes (SWNT) have been investigated using the G6-1 powder diffractometer at LLB [1]. Hydrogen-deuterium substitution in THF allows a layered structure around the nanotubes to be determined. The important changes in the neutron diffraction profile of ternary compounds by comparison with pristine SWNT (figure a) can be understood and simulated assuming that the alkali cations form a monolayer surrounding each tube of the bundle, while THF molecules intercalate between the decorated tubes and at the surface of the bundles (figure b). The structural model we propose also allows to state that the vanishing of the diffraction feature at  $0.6\ \text{\AA}^{-1}$  in the  $\text{LiC}_{5.88}$ -TDF compound is integrally due to isotopic contrast effects, the structure of both hydrogenated and deuterated compounds remaining exactly the same. In spite of this insertion, the triangular bundle structure is preserved, albeit with a much larger lattice parameter, which depends on the size of the inserted cation.

[1] J. Cambedouzou et al., Phys. Rev. B **72** (2005), 041404(R)

[Collaboration : J. Cambedouzou, S. Rols, N. Bendiab, R. Almairac and J.L. Sauvajol (LCVN Montpellier), P. Petit and C. Mathis (ICS Strasbourg), I. Mirebeau (LLB Saclay), M. Johnson (ILL Grenoble)]



**Figure :** a) Experimental (plain lines) and calculated (dotted lines) neutron diffraction profiles of hydrogenated (top) and deuterated (center) ternary compounds, and pristine SWNT (bottom). b) Representation of a  $\text{LiC}_6$ -THF bundle of seven tubes.