



Contribution ID: 45

Type: oral presentation

## Hydrogen in AB<sub>2</sub> and AB<sub>5</sub> compounds

Thursday 6 July 2017 13:20 (20 minutes)

Hydrogen is seen as one of the important energy carriers of this century and is indicated as a fuel of future. Research problem of physical properties of metal hydrides is strongly connected with very actual topical issues of the hydrogen storage. Especially interesting and promising are hydrides of intermetallic compounds. Among widely studied RT<sub>2</sub>H<sub>x</sub> systems (R a rare earth or alkaline metal, T –transition metal like Fe, Co, Ni and Mn), the hydrides RMn<sub>2</sub>H<sub>x</sub> present very interesting physical properties. It comes from the fact that already alone RT<sub>2</sub> compounds exhibit a complex interaction of two sublattices: the R- and 3d-metal sublattice. The first one can be described with the localized 4f magnetic moments, while the other is regarded as essentially an itinerant electron system.

The RMn<sub>2</sub> compounds can absorb very easily large amount of hydrogen, which locates inside of characteristic tetrahedrons build of R and Mn atoms. The systematic investigation (XRD, ND and magnetic measurements) of the RMn<sub>2</sub>H<sub>x</sub> hydrides with R = Y, Nd, Sm, Gd, Tb, Dy, Ho and Er allowed to observe the role of rare earth metal in hydrogen induced structural and magnetic transformations. Hydrogen absorption in RMn<sub>2</sub> compounds leads to magnetic and structural changes: an increase of the magnetic ordering temperature - from below 100 K up to (200 ÷ 400) K depending on the hydrogen concentration, structure transformations and an increase of the cell volume (even up to 30 %).

The role of the host structures (Laves phases of the C14 and C15 type) in formation of hydrides and their magnetic properties is presented –on the base of obtained results the universal structural phase diagram model of RMn<sub>2</sub>H<sub>x</sub> is proposed. It is shown that all the RMn<sub>2</sub>H<sub>x</sub> hydrides in magnetic ordering state are ferrimagnetic and their total magnetization strongly depends on hydrogen concentration. A modified model describing the changes of unit-cell volume as a function of the hydrogen concentration is proposed.

The AB<sub>5</sub> compounds (the most famous representative is LaNi<sub>5</sub>) also easily absorb hydrogen. In comparison to AB<sub>2</sub> the AB<sub>5</sub> absorb and desorb hydrogen at “ambient” temperature and pressure. It is strongly important when we have biohydrogen from bioreactors available. It turns out that small admixtures of selected elements can significantly change the thermodynamic parameters of the host LaNi<sub>5</sub> compound, which is important for the design of hydrogen storage facilities. The last results of *p**c**T* (pressure-concentration-temperature) investigations for LaNi<sub>5</sub>X will be presented as well.

### Acknowledgements

The presented results were partly funded by the project BIOSTRATEG2/297310/13/NCBR/2016.

**Author:** Dr BUDZIAK, Andrzej (Department of Soft Matter Research, Institute of Nuclear Physics PAS, Kraków, Poland)

**Co-authors:** Dr DEBSKI, Adam (2Institute of Metallurgy and Materials Science Polish Academy of Sciences, 25 Reymonta St., 30-059 Krakow, Poland); Mr LODZIANA, Zbigniew (Department of Structural Research, Institute of Nuclear Physics PAS, Kraków, Poland)

**Presenter:** Dr BUDZIAK, Andrzej (Department of Soft Matter Research, Institute of Nuclear Physics PAS, Kraków, Poland)

**Session Classification:** Computational Physics

**Track Classification:** Miscellany (biologically oriented systems, new ideas, advanced methods,...)