

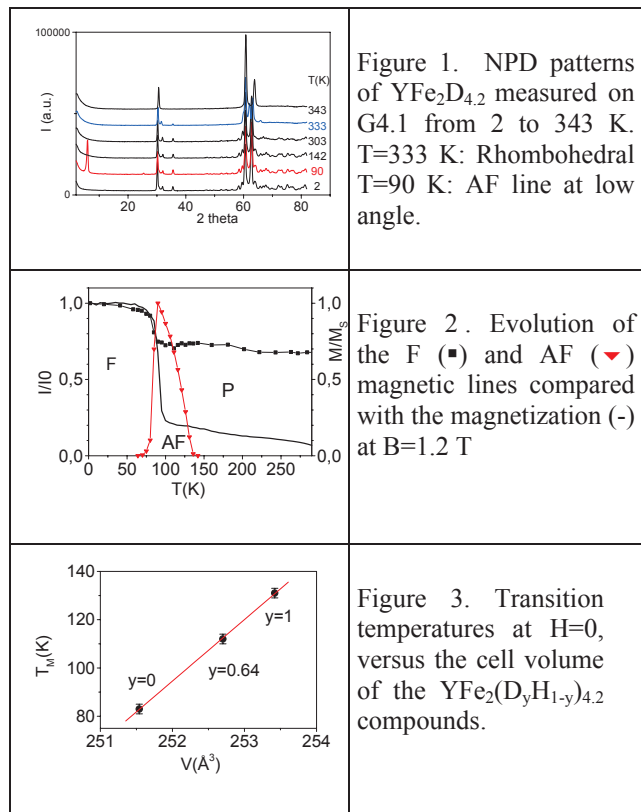
GIANT H/D ISOTOPIC EFFECT IN $\text{YFe}_2(\text{H}_y\text{D}_{1-y})_{4.2}$ COMPOUNDSV. Paul-Boncour¹, M. Guillot², G. André³, F. Bourée³, G. Wiesinger⁴, A. Percheron-Guégan¹¹ LCMTR, CNRS, 2 rue H. Dunant, 94320 Thiais Cedex, France² LCMI, CNRS-MPI, BP166, 38042 Grenoble Cedex 9, France³ LLB, CE-Saclay, 91191 Gif/ Yvette, France⁴ IFP, T.U. Wien, Wiedner Hauptstrasse 8-10, 1040 Vienne, Autriche

Hydrogen absorption in RM_2 ($R=\text{Y}$, Rare earth, $M=\text{Mn, Fe, Co}$) Laves phase compounds has been widely studied due to its strong effect on the electronic and magnetic properties of these compounds [1]. In YFe_2D_x deuterides, D absorption leads to a decrease of the Curie temperature and an increase of the mean Fe moment up to $x=3.5$ [2]. For $x=5$ a strong decrease of the Fe moments occurs, due to a predominant effect of the Fe-D bonding, which shift the Fe 3d band towards the valence band and leads to a strong decrease of the DOS at the Fermi level [3]. $\text{YFe}_2\text{D}_{4.2}$, which lies in the range of magnetic instability, displays a sharp first-order magnetic transition from a ferromagnetic state to low magnetic state at 83 K. Neutron powder diffraction (NPD) experiments were performed on 3T2 and G4.1 to determine both the nuclear and magnetic structures of $\text{YFe}_2\text{D}_{4.2}$. From 343 down to 303 K, a progressive lowering of the crystal symmetry from cubic (C15) to rhombohedral and then monoclinic structure is observed (Fig. 1). At 303 K $\text{YFe}_2\text{D}_{4.2}$ crystallizes in a primitive monoclinic space group P1c attributed to D order. This lowering of crystal symmetry leads to very different D neighbours distribution around each Fe site: 3.2 D for Fe1, 4.4 D for Fe2 and 5.2 D for Fe3. This nuclear structure remains down to 2 K, but a 0.55 % increase of the cell volume is observed around 90 K for the deuteride [4-5]. From 80 K to 132 K additional antiferromagnetic (AF) lines can be indexed with a doubling of the cell along b (Fig.1 and 2). Below 80 K, these AF lines disappear and a ferromagnetic (F) order is observed down to 2 K (Fig. 2). With the support of Mössbauer spectroscopy, the F-AF transition can be attributed to the collapse of the Fe3 moment which is close to the ferromagnetic instability. Above the F-AF transition, the magnetization curves show an

itinerant electron metamagnetic (IEM) behaviour as observed in RCO_2 compounds [6].

A partial or complete substitution of deuterium by hydrogen atom leads to a linear increase of the transition temperature from 83 up to 131 K (extrapolated at $H=0$) and to an increase of $0.4 \mu\text{B}$ of the saturation magnetization at 4.2 K.

$\text{YFe}_2(\text{D}_y\text{H}_{1-y})_{4.2}$ compounds have the same monoclinic structure than $\text{YFe}_2\text{D}_{4.2}$ ($y=1$) at 290 K, but the cell volume of the hydride is 0.75 % larger than for the deuteride due to strong zero point vibration effect. This cell volume expansion can explain the large isotopic effect (Fig. 3), since it has been observed for other IEM compounds that a volume increase stabilizes the ferromagnetism [7].



References

1. G. Wiesinger, G. Hilsher. Topics in Applied Physics. L. Schlapbach. Berlin, Springer-Verlag. **63** (1988) 285
2. V. Paul-Boncour, A. Percheron-Guégan, J. Alloys Comp., **293-295** (1999) 237
3. V. Paul-Boncour, S. Matar, Phys. Rev. B, (2004) in press
4. V. Paul-Boncour, G. André, F. Bourée, M. Guillot, G. Wiesinger, A. Percheron-Guégan, Physica B, **350**, 2004, e27
5. V. Paul-Boncour, M. Guillot, G. G. André, F. Bourée, G. Wiesinger, A. Percheron-Guégan, J. Alloys Comp. (2004) submitted
6. D. Gignoux and D. Schmitt, Handbook of the Physics and Chemistry of Rare Earths. J. Gschneidner, K. A. and J. a. L. Eyring Eds., Elsevier Science B.V. **20** (1995) 293
7. H. Wada, K. Yoshimura, G. Kido, M. Shiga, M. Mekata, Y. Nakamura, Solid State Comm., **65** (1988) 23