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Effect of hydrogen as interstitial element on the magnetic properties of iron rich intermetallic compounds: the case of YFe_2

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Abstract. Surprisingly, hydrogen which is a non magnetic element, is known to induce dramatic modification of the magnetic properties of intermetallic compounds made of rare-earth and transition metal elements [1-2]. This effect has for long time remained a curiosity and motivated fundamental research mainly however new applications of such intermetallic magnetic hydrides are now discussed worldwide. An introduction will present the effects of hydrogen insertion on the intrinsic magnetic properties of iron rich intermetallic compounds. We will shortly review the main effects of hydrogen insertion on the magnetization, type of magnetic ordering of these intermetallic compounds. Then we will mention the potential use of such hydride systems for new applications. Selecting the example of YFe_2H_x system we will describe in more details recent work on the hydrogen induced modifications of the structural properties including crystal and magnetic ones [3]. YFe_2 can absorb up to 5 H or D atom/f.u. and a large variety of crystal structure is observed as a function of H content. $YFe_2D_{4.2}$ exhibit a monoclinic structure at ambient temperature and pressure, related to a distortion of the initial cubic C15 structure of YFe_2 by the ordering of inserted D atoms [4]. This compound presents remarkable magnetic properties which are found to be very sensitive to the volume change induced by H for D substitution or chemical substitution. In order to understand this unusual behavior, we present the study of the structural and magnetic properties of $YFe_2D_{4.2}$ under high pressure by combining energy dispersive X-ray diffraction performed at RT up to 5.5 GPa, neutron diffraction studies at low temperature up to 2.5 GPa and magnetization measurements up to 1 GPa [3]. A structural transition from monoclinic to cubic structure is observed at 4 GPa. The high pressure cubic $YFe_2D_{4.2}$ has a 19 % higher cell volume than that of YFe_2. At 84 K and ambient pressure, a transition from a ferromagnetic to an antiferromagnetic structure is accompanied by a jump of volume (0.65 %). The ferromagnetic order disappears above $P = 0.54$ GPa, and the antiferromagnetic structure is the only remaining one as observed by neutron diffraction. Using the compressibility value determined by X-ray diffraction ($\kappa = 0.013$ GPa^{-1}), this volume decrease is in very good agreement with the volume contraction (0.70 %) observed at this critical pressure of 0.54 GPa. The pressure evolution of the structural and magnetic phase diagram of $YFe_2D_{4.2}$ has therefore been determined.

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