Poster Th-019

DIRECTIONAL METAL-HYDROGEN BONDING IN INTERSTITIAL HYDRIDES, I - $ErNi_3H_x$ ($0<x<3.7$)

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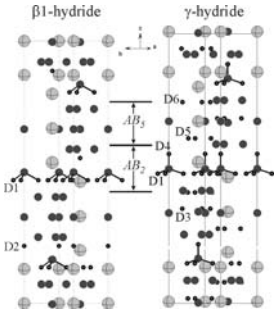

Hydrogenetion of $ErNi_3$ (rhombohedral $PuNi_3$ type structure) has been investigated by synchrotron and neutron powder diffraction. At least three hydride phases were found: β_1: x~1.3; β_2: x~2 and γ: x~3.7, the latter being stable only under hydrogen pressure (~100 bar). While the lattice expands mainly along ***c*** in the β-phases, it expands in the basal plane on transition to the γ - phases. In the β-phase hydrogen enters two types of interstitial sites in the AB_2–type building block (see figure left). One (D1) corresponds to three ligands of a Ni centered NiH_4 tetrahedron, and the other (D2) bridges a Ni triangle. In the γ-phase D2 becomes nearly empty while four other interstitial sites become occupied. One (D4) completes the fourth ligand of the NiH_4 tetrahedron, and three (D3, D5, D6) are located in the AB_5 building block (see figure right). The formation of tetrahedral NiH_4 units suggests directional bonding effects similar to those in complex hydrides such as $LaMg_2NiH_7$ and Mg_2NiH_4. As expected these effects are similar to those in the nickel based analogoue β-$HoNi_3H_x$ but different from those in the cobalt analogues β- and γ-YCo_3H_x. This demonstrates that hydrogen atom distributions in interstitial metal hydrides cannot be rationalized by geometrical considerations alone.