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The Crystal Structure of NdGaDx

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Hydrogen absorbed in alloys is much denser than compressed or even liquid hydrogen.

Most REGa (RE=lanthanide) compounds are reported to crystallise in the CrB-type structure (space group Cmcm). GdGa, with unit cell a=4.3372 b=11.0316 c=4.1106, does, in addition to store hydrogen interstitially, exhibits a magnetocaloric effect and has a Curie temperature at 183K. It is probable that the addition of hydrogen will affect the magnetic properties.

One important aspect in understanding the effect of the addition of hydrogen is solving the crystal structure of GdGaHx. Depending on the interstitial sites occupied, hydrogen atoms can be surrounded by only Gd atoms, by only Ga atoms or in sites in coodinated by both types of atoms. The single electron of H atom makes it, in practice, next to impossible to locate by X-ray diffraction techniques. Neutron diffraction could be used to locate the H atoms; however, the extreme neutron absorption coefficient of Gd is probably an insurmountable obstacle to perform these measurements.

Luckily, there are (as previously mentioned) a large number of iso-structural lanthanide RE-Ga compounds. We have synthesised NdGa and NdGaDx (deuteriude is much more suiteable for neutron scattering due to very high coherent scattering from hydrogen) and propose to solve the structure of NdGaDx by combining X-ray and neutron powder diffraction of NdGa and NdGaDx. The chemical similarities between Nd and Gd should ensure that conclusions about the structure of NdGaDx are mostly valid for GdGaHx.

These measurements will be performed in collaboration with Magnus Sörby at the Institute for Energy Technology, Physics Department in the EU infrastructure project H2FC.