Application 2030

Hydrogen absorption in Nb4Co1-xNixSi

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Nb4CoSi and Nb4NiSi, crystallising with the Al2Cu-type structure, space group I4/mcm, absorb considerable amounts of deuterium at room temperature and 90-kPa deuterium pressure. The deuterium contents for the pure compounds were determined to be Nb4CoSiD2.5 and Nb4NiSiD2.7 from neutron powder diffraction. In the pure compounds, two crystallographic sites, 4b and 16l, are occupied by deuterium to 78.2(6)% and 12.2(3)% in Nb4CoSiD2.5 and 63.6(8)% and 18.6(5)% in Nb4NiSiD2.7. Each deuterium atom coordinates four niobium atoms in a tetrahedral arrangement.

In the proposed project we will investigate samples in the composition range Nb4Co1-xNixSi, $0.1<x<0.9$. These solid solutions are unknown from a hydrogen absorption point of view. Deuterated samples in powder form will be investigated with respect to crystal structure and hydrogen storage properties. Furthermore, the undeuterated samples become superconductors at low temperatures (~7K). The effect of hydrogen/deuterium on the superconducting properties will be evaluated and the low temperature structure will be investigated from low temperature neutron diffraction measurements.

We propose to measure three samples in the composition range Nb4Co1-xNixSi, $0.1<x<0.9$. Furthermore, these samples will be measured with varied hydrogen/deuterium content, giving a total of 6-8 measurements. The samples absorb hydrogen/deuterium readily at room temperature so it would be possible to start from a undeuterated sample and then increase the hydrogen/deuterium content stepwise and investigate structural transitions as a function of hydrogen/deuterium content.

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