Experimental report

12/10/2016

Proposal: 7-03-149 **Council:** 4/2015

Title: Hydrogen diffusion in a Fe/VHc superlattice measured with Quasi-Elastic Neutron Scattering

Research area: Physics

This proposal is a new proposal

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Samples: Fe/(VH0.65) thin film on MgO substrate

Instrument	Requested days	Allocated days	From	To
IN6	0	2	05/07/2016	08/07/2016
IN12	12	0		
THALES	12	0		

Abstract:

We propose to measure hydrogen diffusion in a Fe/VHx [2/14] superlattice with quasi-elastic neutron scattering. Hydrogen is one of the major candidates to replace carbon based fuels with sustainable energy sources. Both thermodynamics and kinetics of hydrogen-metal systems are greatly altered by mechanical influences such as strain, finite size (down to the nano regime) and proximity to interfaces. Single-crystal superlattices, for example Fe/V and Cr/V represent one of the most highly controlled class of model systems to investigate these effects, since they can be grown to high quality and only one of the constituents absorbs hydrogen (vanadium). We have estimated the count rate expected for a hydrogen concentration of c=0.65 H/V and found that an experiment on IN12 or Thales is feasible. Our experiments are the first of its kind on thin films loaded with hydrogen. If they are successful, they will open the door towards a series of studies of diffusion in thin films where effects of finite size, strain engineering and proximity can all be studied.

The scientific question to be addressed was whether a thin film loaded with hydrogen would exhibit detectable elastic, or quasi-elastic, as compared to an identical film in every way except without hydrogen. Since IN6 has such a large detector, the detected signal extends quite far in energy loss beyond the quasi elastic peak. Figure 1a shows data from the two films at 300 K. The data has been divided by the monitor, angle dependent detector efficiency, wavelength dependent efficiency of the detector gas and integrated over angle. The angle dependent detector efficiency was determined from a separate measurement of a vanadium powder at low temperature. Figure 1b shows the same spectra after a time independent background has been subtracted.

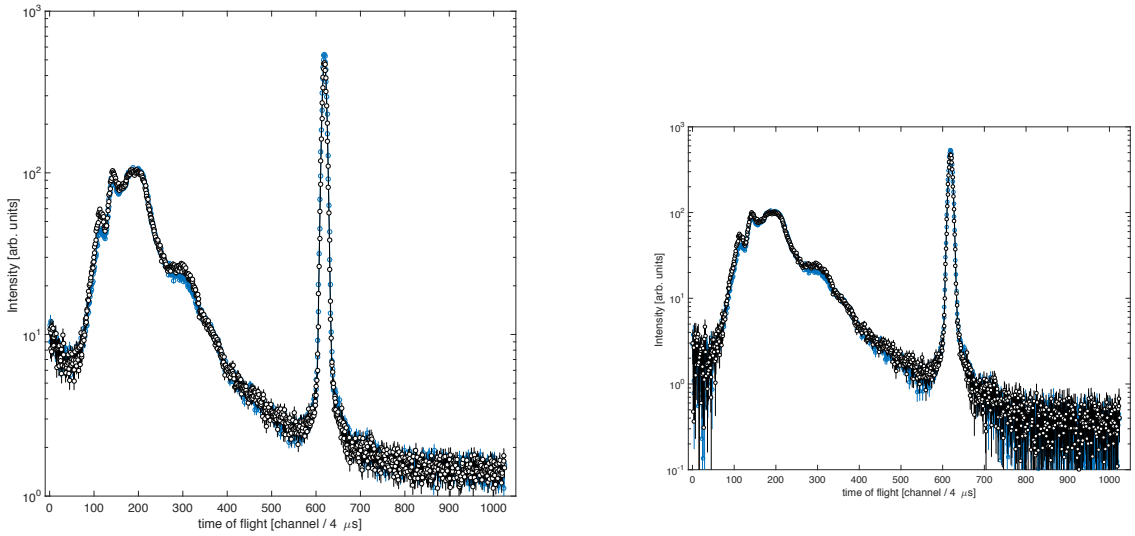

Figure 1. Left panel shows time of flight spectra from V_2H (blue) and V (black) at room temperature. The right panel shows the same spectrum after a time independent background has been subtracted.

There are clear differences in the two spectra that cannot be explained by an artefact of the data reduction procedure. In fact, the elastic peak intensity is larger for the sample loaded with hydrogen. Figure 2 shows part of the spectrum from Fig. 1 (b) on a linear scale. No scaling of the data has been performed at this stage and as can be seen there are parts of the energy spectrum which is identical whereas an intensity redistribution has occured in other parts of the spectrum. The spectrum is a combination of the spectrum from the aluminium windows, the MgO substrate and the film itself. The same sample holder was used at the same incident angle for the two samples. The two films were produced from the same batch of substrates and cut to be of the same size. A difference in sample amount would only result in a uniform scaling of the intensity.

We now proceed with the data reduction and convert time-of-flight to energy transfer, with its associated Jacobian correction as well as the Bredov integration over momentum transfers and thermal occupation numbers, to produce a PDOS, as shown in Fig. 2.

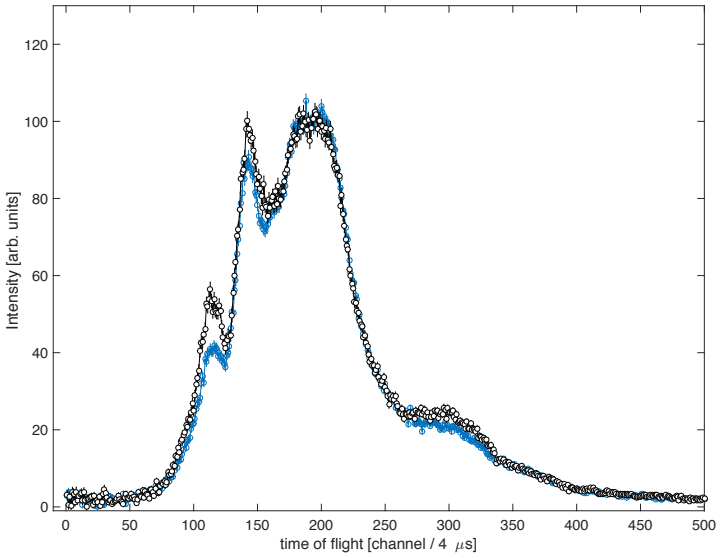

Figure 2.

As can be seen in the figure, which includes a separate bulk vanadium measurement (blue) and a measurement from the empty aluminium sample holder (red). The red solid line is a density functional calculation of the phonon density of states. The black circles represent the difference between the loaded sample and the unloaded sample.

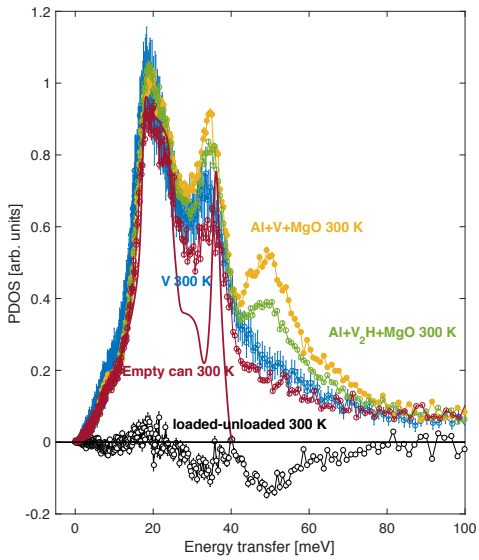

Figure 3.