Electronic Supplementary Information for

Understanding composition-property relationships in Ti-Cr-V-Mo alloys for optimisation of hydrogen storage in pressurised tanks

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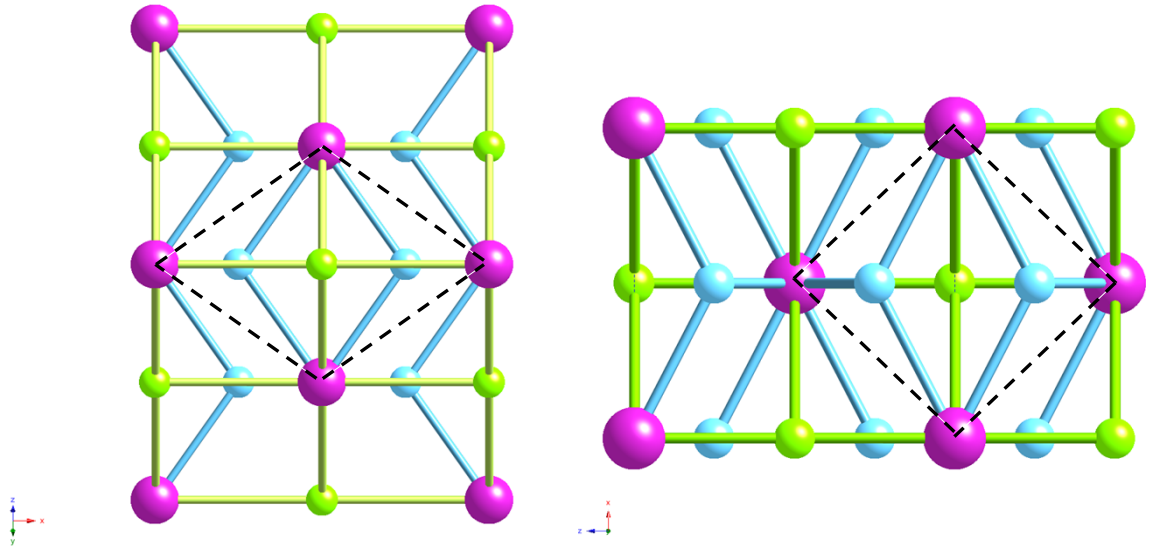
Details on Neutron Powder Diffraction Data Analysis

The Aluminium alloy cell was fitted using the Pawley method. The bct and fcc phases (where present) were refined using the Rietveld method. The unit cell parameters obtained from the X-ray data were used as the initial starting points for the bct and fcc phases. The unit cell parameters, hydrogen site occupancies and phase fractions were refined. A single global thermal parameter was refined for all of the metal hydride atoms in the sample.

	bct	**fcc**
Space group	I4/mmm	Fm-3m
M site Wykoff	2a	4a
1x 10^{-6} bar		
a / Å	3.1302(11)	4.2881(25)
c / Å	3.2136(10)	
c/a	1.0266	
volume	31.488(32)	78.85(14)
Mass %	98.56(73)	1.44 (73)
100 bar		
a / Å	3.1227(14)	4.2836(3)
c / Å	3.2344(15)	
c/a	1.0357	
volume	31.540(19)	78.599(17)
Mass %	1.58(4)	98.42 (4)

Table S1 Unit cell parameters for V_{75} bct and fcc phase from X-ray data (1 cycle sample)



a b

Figure S1 (**a**) fcc viewed down the 011 direction (**b**) bct phase viewed down b (extended ½ a unit cell along c) and with sites H11 and H22 not shown. Metal atoms are shown in pink, octahedral sites in green, tetrahedral sites in blue.

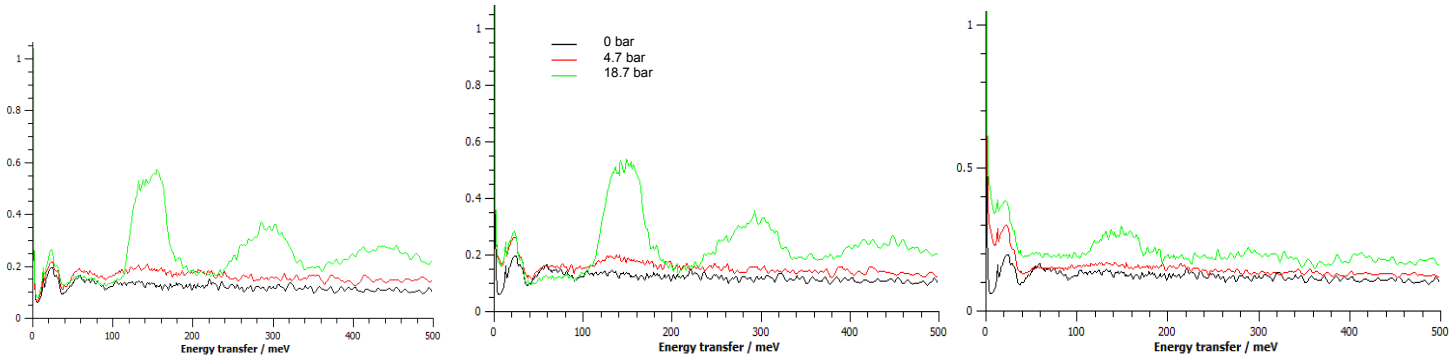


Figure S2 Effect of temperature at (**a**) 4K, (**b**) 200K and (**c**) 300K on peak shape and intensity in INS spectra for V_{20} 10 cycles across various hydrogen P_{eq}.

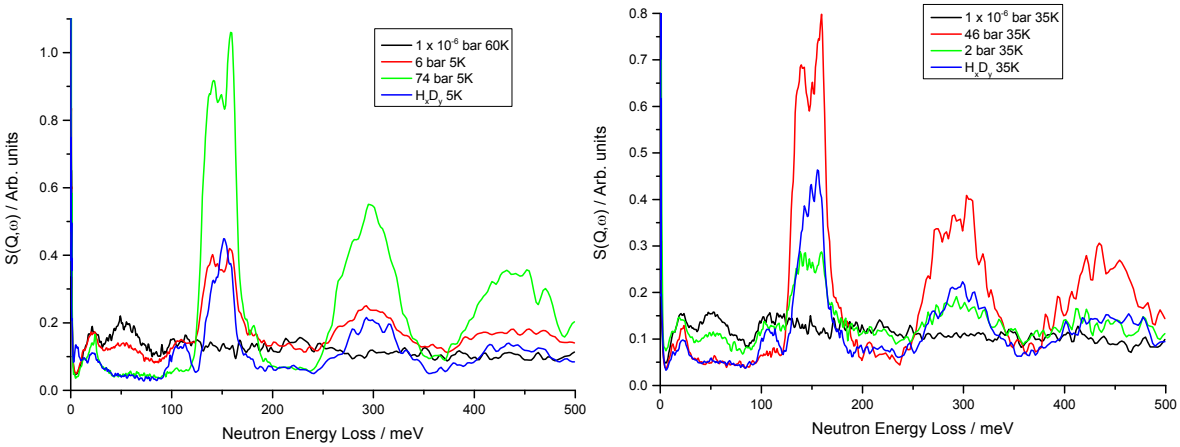


Figure S3 Addition of deuterium to V_{75} (**a**) 1 cycle and (**b**) 10 cycle samples.

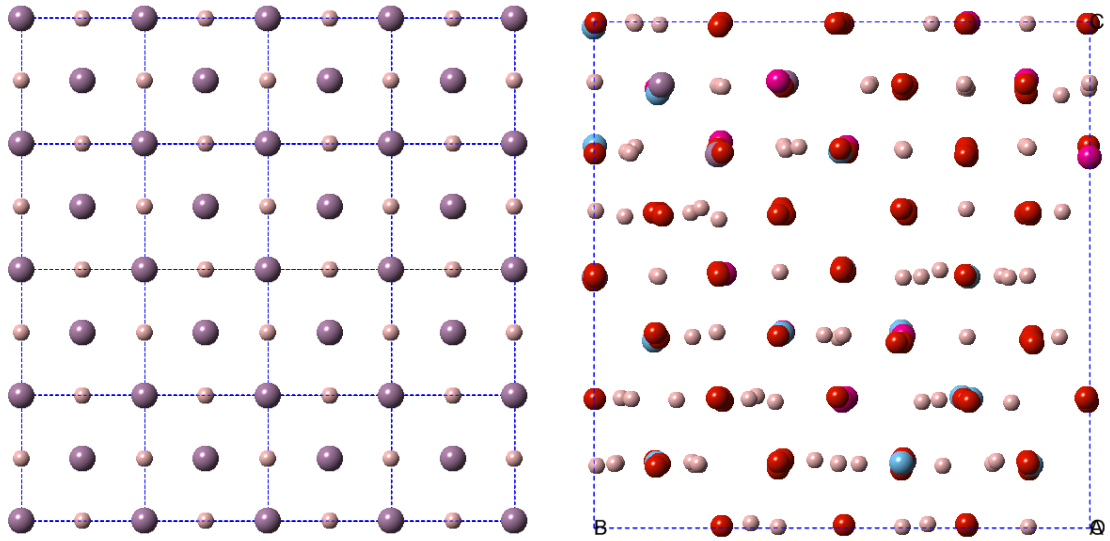


Figure S4 (**a**) Expansion of the unit cell for the bct phase obtained from NPD data with hydrogen on the Oz site and (**b**) equivalent 4 x 4 x 4 supercell generated in CASTEP with the correct atomic ratio of Ti-Cr-V-Mo atoms and structure relaxation performed resulting in a disordered arrangement from their special positions. Both viewed down the *a* axis.