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Hydrogen Diffusivity Measurements of $YH_{1.87}$ Moderator Material with Incoherent Quasielastic Neutron Scattering

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Transformational Challenge Reactor Program

HYDROGEN DIFFUSIVITY MEASUREMENTS OF $YH_{1.87}$ MODERATOR MATERIAL WITH INCOHERENT QUASIELASTIC NEUTRON SCATTERING

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ACRONYMS

Al	aluminum
CaF_2	calcium fluoride
DAVE	Data Analysis and Visualization Environment
DOE	US Department of Energy
FCC	face-centered cubic
Gd	gadolinium
H	hydrogen
HCP	hexagonal close packed
HWHM	half width at half maximum
IQNS	incoherent quasielastic neutron scattering
La	lanthanum
LaH_2	lanthanum hydride
NMR	nuclear magnetic resonance
ORNL	Oak Ridge National Laboratory
Pt	platinum
Sc	scandium
ScH_2	scandium hydride
TCR	Transformational Challenge Reactor
$Th\text{-}ZrH_x$	thorium zirconium hydride
TiH_x	titanium hydride
$U\text{-}ZrH_x$	uranium zirconium hydride
V	vanadium
XRD	x-ray diffraction
Y	yttrium
YH_x	yttrium hydride
YH_2	yttrium dihydride
YH_3	yttrium trihydride
ZrH_x	zirconium hydride

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ABSTRACT

Yttrium hydride is an optimal choice of moderator material for thermal neutron spectrum reactors requiring small core volumes. The Transformation Challenge Reactor (TCR) program at Oak Ridge National Laboratory (ORNL) aims to develop an additively manufactured microreactor core by leveraging recent advances in materials, manufacturing, data analytics, and high-fidelity modeling and simulation. Yttrium hydride was selected as the moderator material for TCR due to its high moderating power, which enables the spatially efficient reactor design and thermal stability that is superior when compared with zirconium hydride. Hydrogen desorption from yttrium hydride is expected at elevated temperatures, posing safety and performance concerns. As a lifetime component in advanced reactors, appropriate strategies to mitigate hydrogen release from yttrium hydride over long-term reactor operation are required. Understanding hydrogen mobility in yttrium hydride provides the scientific basis for developing a hydrogen barrier for hydride moderator and predicting the hydrogen redistribution within the material during various operational conditions. This study investigated the hydrogen motion in $YH_{1.87}$ as a function of temperature ranging from 200 to 1,173 K using incoherent quasielastic neutron scattering (IQNS) at the Spallation Neutron Source (SNS). The results are presented and discussed in terms of hydrogen self-diffusion coefficients, activation energy for translational hydrogen motion, and hydrogen jump distances. Based on the IQNS data, $YH_{1.87}$ is found to be stable at high temperatures with no translational H motion below 1,023 K within the IQNS detection limits. In the temperature range of 1,073–1,173 K, hydrogen diffusivity in $YH_{1.87}$ is $D = 4.57 \times 10^{-3}[m^2/s] \exp\left(-\frac{1.73\ [eV]}{RT}\right)$. The hydrogen concentration's dependence on hydrogen diffusivity is also discussed in this report.

1. INTRODUCTION

By reason of its substantial equivalence in mass to neutron and its acceptably high scattering cross section, hydrogen is an outstanding neutron energy degrader for neutrons of less than a few MeV kinetic energy via elastic collision. The neutron-moderating characteristics of hydrogen are very useful for bringing the incident neutron energy to a level at which it has a greater probability of interaction with other atoms; that is, fissile, fertile, and neutron-poison atoms. Therefore, hydrogen-bearing materials are commonly used as moderators in thermal neutron spectrum reactors. Transition metals are known to absorb large quantities of hydrogen to form a hydrogen solid solution at low hydrogen content, and they form hydrides at higher hydrogen content. The densities of hydrogen atoms in some transition metal hydrides are greater than those in water or in liquid hydrogen, thus enabling a variety of applications within nuclear and non-nuclear systems [1].

Metal hydrides have been considered as optimal moderator options for advanced nuclear reactors. Some advanced reactor designs [2] call for increased thermal efficiencies and thus, higher operating temperatures. Although H_2O has been widely used as the moderator in light-water reactors, its application as a high-temperature (>400°C) moderator material is restricted by the requirement for extremely high pressure. In contrast, various metal hydrides can maintain hydrogen density to temperatures greater than 500°C [3]. For example, the use of ZrH_x as a high-performance moderating material in advanced reactors is a design option used repeatedly [4-6]. Fuel-moderator combinations are commonly researched subjects, as in U-ZrH_x [5] and Th-ZrH_x [7]. Among these combinations, Simnad [5] claims that ZrH_x with $x\approx2$ can be used at temperatures as high as 750°C, where ZrH_2 maintains a hydrogen atom density (N_H) equivalent to water, in equilibrium with 1 atm of H pressure. However, this value rapidly decreases thereafter, and it plummets at temperatures higher than 900°C [3]. In contrast, YH_x exhibits superior thermal stability. For example, when in equilibrium with 1 atm of hydrogen, YH_x remains stable at temperatures greater than 1,000°C [3]. It is noted that the neutron absorption cross section of yttrium is 6 times that of zirconium.

The US Department of Energy (DOE) Office of Nuclear Energy launched the Transformational Challenge Reactor (TCR) program at Oak Ridge National Laboratory (ORNL) in 2019 to demonstrate a faster, more affordable approach to advanced nuclear energy [8, 9]. Yttrium hydride has been chosen as the moderator material for TCR [8]. ORNL has successfully demonstrated fabrication of crack-free, bulk yttrium hydride and has initiated a campaign to develop a comprehensive, reliable database of yttrium hydride [10]. Of particular concern is the hydrogen desorption from metal hydride at elevated temperatures when in service in reactors [7, 11], altering the criticality condition of the reactor and potentially inducing embrittlement in other components, posing significant performance and safety concerns. Mitigation strategies must be developed to maintain the required amount of hydrogen for metal hydride as a lifetime component over the reactor's operational lifetime. Hydrogen barriers to be developed include metal cladding with low hydrogen permeability, glass-coated metal cladding, and self-protecting oxide or nitride layers that are included directly on the hydride's surface [12]. The development of hydrogen barriers for yttrium hydride relies on the fundamental understanding of hydrogen mobility across the hydride. In addition, the fabrication process of high-quality yttrium hydride will also be informed by the hydrogen mobility study, through which the processing temperature and duration can be optimized. Stuhr et al. [13] report that the migration energy for self-diffusion of hydrogen in $YH_{1.97}$ is 0.3 eV. This was determined by performing the incoherent quasi-elastic neutron scattering (IQNS) experiments. This is the only available relevant data, as determined from the yttrium hydride powders fabricated through introducing a known amount of hydrogen. However, this method is considered unreliable for determining hydrogen concentration. This research relied on the high-quality yttrium hydride fabricated from the TCR program to study hydrogen mobility. The incoherent neutron scattering cross section of hydrogen is the second largest in the periodic table, following Gd, making IQNS the ideal tool for detecting localized and translational hydrogen motion in the lattice. IQNS has been used to detect hydrogen motion in a variety of materials [7, 13-15] down to very low hydrogen concentrations (e.g., $ZrH_{0.0155}$ [16]).

This report presents results from a detailed study on hydrogen motion in $YH_{1.87}$ moderator material using IQNS within the temperature range of 200–1,173 K. Within this context, quasi-elastic line broadening is used as a function of temperature to determine hydrogen self-diffusion coefficients, H jump distances, and translational jump times.

2. EXPERIMENTS

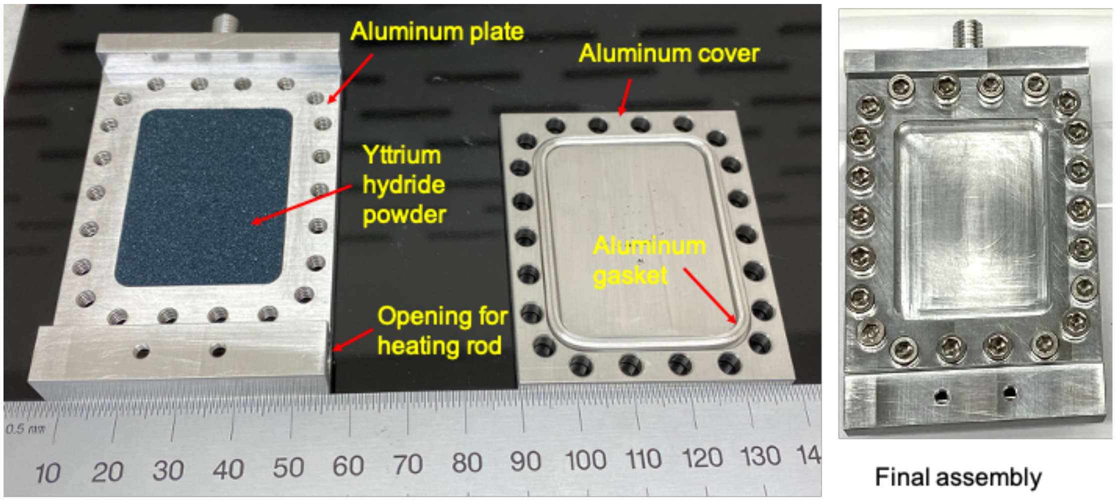
2.1 YTTRIUM HYDRIDE MANUFACTURING

Yttrium hydride samples with an H/Y atomic ratio of 1.87 were fabricated through direct interaction of ultra-high purity metallic yttrium (nominal 99.99%, purchased from American Elements) and hydrogen at elevated temperatures. Carefully matching the processing temperature and the hydrogen partial pressure in the retort gives rise to the desired hydrogen concentration as informed by the well-established thermodynamics of the Y-H binary system. More details regarding fabrication of yttrium hydride are available in a recent paper by Hu et al. [10]. The hydrogen stoichiometry of the synthesized specimens was determined using the weight change method. X-ray diffraction (XRD) measurement was also performed to identify the phases presented within the samples. The results showed that both alpha-yttrium and delta-yttrium hydride were found in the fabricated hydride samples. The fabricated $YH_{1.87}$ contained 97.6 wt% delta-yttrium hydride and 2.4 wt% alpha-yttrium at room temperature.

2.2 HYDROGEN DIFFUSIVITY MEASUREMENTS WITH IQNS

IQNS measurements were carried out at a near-backscattering neutron spectrometer BASIS [17] at ORNL's Spallation Neutron Source, providing an energy resolution of ca. 3.7 μeV (FWHM) and a usable range of energy transfers of -100 μeV to +100 μeV. Two separate sets of measurements were performed at two different beam times. For the measurements at $T \leq 700$ K, henceforth known as *low temperature measurements*, a closed cycle refrigerator (CCR) was used. The IQNS was recorded at seven temperature points: 200, 300, 400, 500, 600, 650 and 700 K. For the measurements at $T \leq 1,173$ K, henceforth known as *high temperature measurements*, a MICAS furnace was used. A temperature interval of 25 K was applied. The instrument resolution functions were collected at ~10 K for the low-temperature measurements and at 300 K for the high-temperature measurements. A momentum transfer (Q) range of 0.3 to 1.9 $Å^{-1}$ was used for both measurements. Both experiments were performed under high vacuum conditions. Data reduction and analyses were performed using the Data Analysis and Visualization Environment (DAVE) software [18].

Powder samples were used for the low-temperature measurements. Bulk yttrium hydride rod (10 mm in diameter and 15 mm in height) with a H/Y ratio of 1.87 was fabricated first and then was crushed and ground into fine powder. To mitigate hydrogen release at elevated temperatures, an Al sample holder was used to contain the powder sample; Al was used because it is almost entirely a coherent scatterer of neutrons. The Al sample holder consists of a plate and a cover (Al-6063). A specially designed Al gasket was used to enable the gas-tight sealing of the final assembly. The yttrium hydride powder was loaded in the volume of 30 mm × 40 mm × 0.5 mm. Figure 1 shows the pictures of the parts for sample holder assembly.



Final assembly

Figure 1. Sample holder parts and final assembly for low temperature measurement.

For the high-temperature experiments, a thin-wall, low boron quartz tube (0.46 mm wall thickness, 9.07 mm inside diameter) was used to contain a 0.11 mm yttrium hydride foil. The ~0.1 mm metallic yttrium foil was first loaded into the quartz tube, and then the assembly was placed in the retort of the TCR bulk metal hydriding system for hydrogen loading. Following the successful fabrication of yttrium hydride foil, the quartz tube was sealed. During the IQNS measurements, the sealed quartz tube containing yttrium hydride foil was placed in a vanadium sample holder connected to the BASIS furnace. Figure 2 shows a picture of the thin wall quartz tubes containing metallic yttrium foil and yttrium hydride foil.

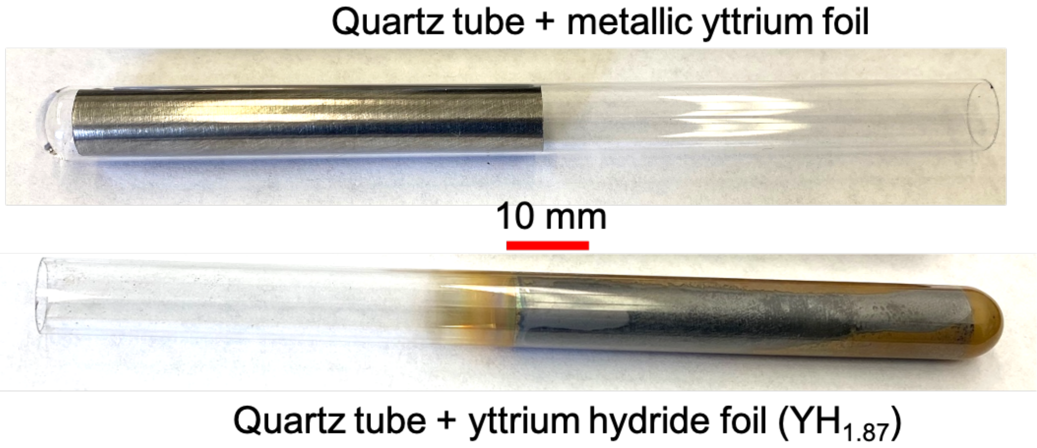


Figure 2. Quartz tube containing yttrium foil and yttrium hydride foil.

2.3 HIGH-TEMPERATURE XRD MEASUREMENTS

The high-temperature x-ray diffraction measurements were performed using a Panalytical X'Pert Pro diffractometer (using CuK$_{\alpha}$ radiation, λ=1.540598 Å) with the XRK 900 oven-type furnace. A parallel beam setup was used to eliminate any peak shifts that could result from sample surface displacement due to volumetric expansion. Helium gas was used to provide an inert atmosphere. Rietveld refinements were performed using Jade 2010 software.

3. RESULTS

To obtain translational diffusivity, the quasi-elastic spectra were fitted using a Lorentzian quasi-elastic term, an elastic term, and a background term. Quasi-elastic line broadening was obtained from the Lorentzian term and expressed using the half-width-at-half-maximum (HWHM) values of the fits. For low-temperature IQNS experiments, no obvious linewidth broadening of the recorded quasi-elastic spectra was observed. Figure 3 shows the HWHM evolution as a function of Q from the low temperature measurements (200~700 K). The HWHM values show no Q dependence, so hence there was no translational motion of hydrogen in yttrium hydride in the studied temperature range, 200~700K.

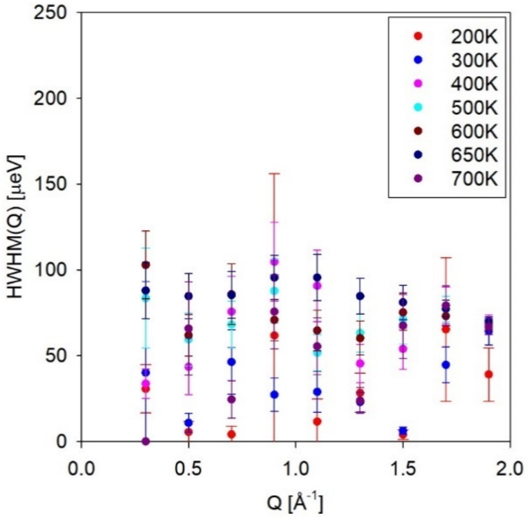


Figure 3. The quasi-elastic linewidth (HWHM) evolution as a function of Q for the $YH_{1.87}$ sample in the temperature range 200K-700K.

The high-temperature quasi-elastic spectra are presented in Figure 4 for Q values of 0.7 and 1.3 as examples for 3 temperatures: 1,073, 1,123 and 1,173 K. Figure 4 reveals the presence of quasi-elastic linewidth broadening indicative of translational motion, which becomes more evident with increasing temperature. No translational motion was observed below 1,073 K.

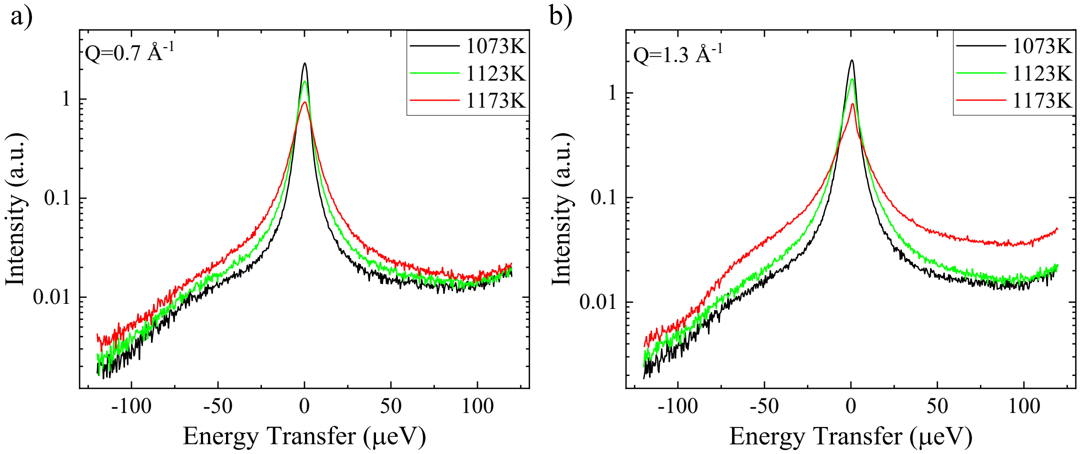


Figure 4. Quasi-elastic spectra for the $YH_{1.87}$ sample at various temperatures (1073 K, 1123 K, 1173 K) for Q values of (a) 0.7 Å^{-1} and (b) 1.3 Å^{-1}.

The evolution of the HWHM values as a function of Q from the high-temperature measurements are presented in Figure 5, which shows a clear evolution of HWHM values as a function of Q for all temperatures.

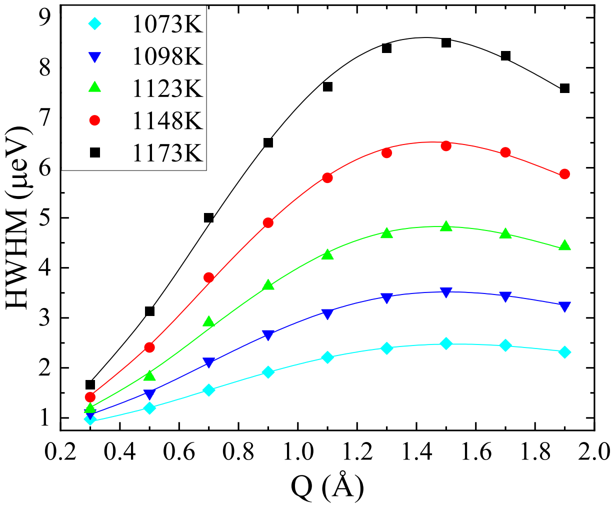


Figure 5. The quasi-elastic linewidth (HWHM) evolution as a function of Q for the $YH_{1.87}$ sample in the temperature range of 1,073–1,173 K. Solid lines correspond to fits using the isotropic Chudley-Elliott model.

Next, the high-temperature HWHM data were fitted using the isotropic Chudley-Elliott model [19] for hydrogen diffusion, as shown in Eq. (1), with a fixed background term:

$$HWHM = \frac{6\hbar D}{l^2}\left(1 - \frac{\sin(Ql)}{Ql}\right), \tag{1}$$

where ħ is the reduced Planck's constant, l is the jump distance, D is the diffusion coefficient, and Q is the momentum transfer. The diffusivity data are then presented in Figure 6 as a function of temperature (1,000/K).

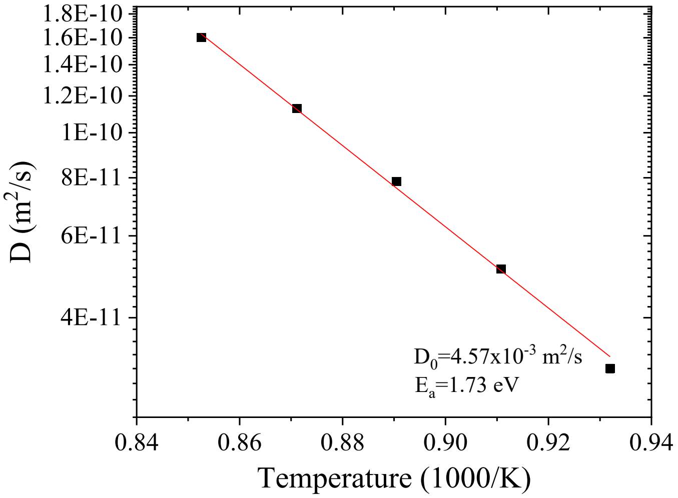


Figure 6. Hydrogen diffusivity values for $YH_{1.87}$ presented as a function of temperature (1,000/K): also shown is the Arrhenius fit to the data following Eq. (2).

The diffusivity follows an Arrhenius-type relation and was fitted using Eq. (2), where E_a is the activation energy, R is the ideal gas constant, T is the temperature, and D_0 is a temperature-independent constant.

$$D = D_0 \exp\left(-\frac{E_a}{RT}\right). \tag{2}$$

The fitting parameters obtained from the plot in Figure 6 are D_0 of 4.57×10^{-3} m^2/s and E_a of 1.73 eV. The activation energy is a term that signifies the energy required to overcome the jump barrier: the higher the energies, the more tightly bonded the H atoms.

Next, in Figure 7, the jump distances (a) and their associated translational jump times (t) (b) are presented. The jump times are derived from the diffusivity following the relation: $t=l^2/D$. Within the studied temperature range, an average jump distance of 3.04 Å is observed.

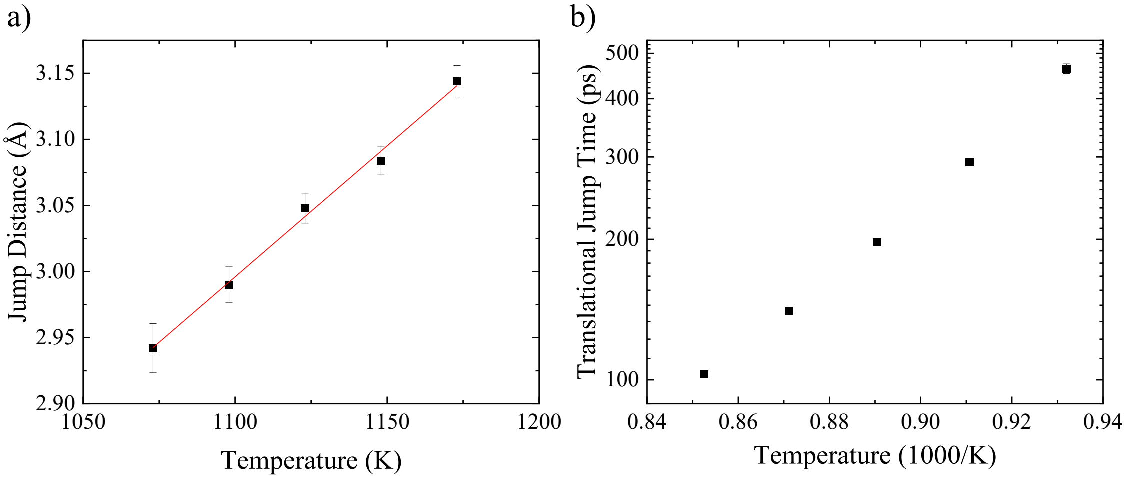


Figure 7. Hydrogen jump distances (a), and translational jump times (b) obtained from IQNS measurements for $YH_{1.87}$.

4. DISCUSSION

The H locations and diffusion mechanisms in metal hydrides have been discussed at length in the literature, and a summary of information related to the H motion in YH_x is presented at the beginning of this section.

The face-centered cubic (FCC) YH_2 phase has the CaF_2 prototype structure [20, 21], where the Y atoms occupy the face centers and corners of the unit cell, and the H atoms can occupy the tetrahedral and octahedral interstitial sites within the lattice [22]. H atoms prefer to occupy the lower energy tetrahedral locations, and it was initially believed that in the dihydride configuration, all the H atoms would be in the tetrahedral sites [21], which when fully loaded would yield Y_4H_8, which is the stoichiometric ratio YH_2. However, it was later shown that octahedral sites are partially occupied before the tetrahedral sites are completely filled at $x<2$ [22-24]. Similar observations were made by Khodosov and Andrievskii [25] in FCC ZrH_2. Interestingly, Peterman et al. [26] reports that while octahedral site occupancy is observed in YH_2 and LaH_2, ScH_2 did not show this behavior, and this possibly related to the lattice constant of the parent element/lattice, which follows as La>Y>Sc, where Sc with the smaller lattice constant does not allow H movement into the octahedral sites.

The site occupancy is dependent on temperature and concentration. When working with $YH_{1.98}$, Khatamian et al. [27] observed a lower H octahedral site occupancy at 11 K than at 300K and suggested that this was related to the migration of H atoms to higher energy octahedral sites with thermal activation. On the other hand, Goldstone et al. [23] studied the site occupancy of $YH_{2.0}$ between 15–420 K and demonstrated that octahedral occupancy tended to decrease with increasing temperature, which was contrary to what was expected. Regarding H concentration dependence, Anderson et al. [28] notes an O-site occupancy increase from 10.5 to 15.5% in $YH_{1.98}$ compared to that of $YH_{1.92}$, as well as hydrogen diffusion rates 3 orders of magnitude higher in $YH_{1.98}$ than in $YH_{1.63}$. On the other hand, Stuhr et al. report an opposite behavior for TiH_x [13], in which increasing x from 1.59 to 1.86 caused the self-diffusion coefficient to decrease. This was related to the lack of O-site occupancy in this material (only T-sites were occupied). Stuhr et al. also studied YH_x with $1.59<x<2.09$ and found increasing self-diffusion coefficient values with increasing x for a given temperature, which was related to the availability of O-sites. Terrani et al. [7] have also measured hydrogen diffusivity and jump distances in two different stoichiometries of the same compound—namely $ThZr_2H_{5.6}$ and $ThZr_2H_{6.2}$—revealing lower self-diffusion coefficient at lower H concentration. However, in this case, the lower self-diffusion coefficient was related to the H atoms being more tightly bonded in $ThZr_2H_{5.6}$, so they required a higher activation energy to overcome the jump barrier.

To understand the active jump mechanism, the possible hydrogen locations in the lattice and the lattice constants at the studied temperatures must be known. The change in lattice parameters due to thermal expansion is presented in Figure 8 and was obtained from in-situ high-temperature XRD measurements on $YH_{1.87}$.

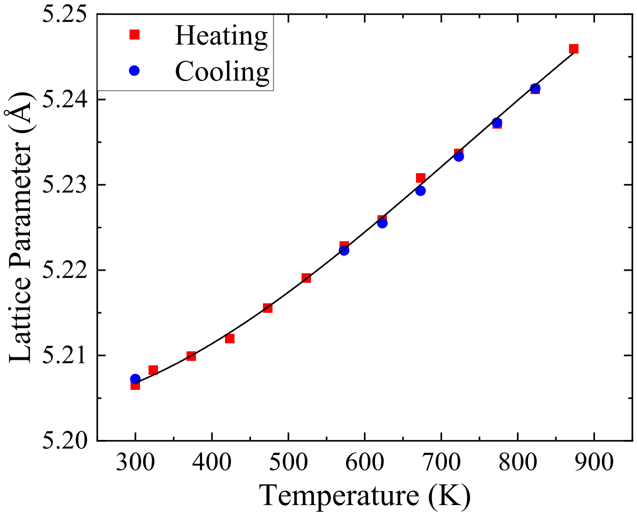


Figure 8. Lattice parameter evolution as a function of temperature for $YH_{1.87}$.

Here, the measurements were performed up to 873 K, and extrapolation was performed to higher temperatures to calculate the expected lattice parameters. The extrapolated data suggested an average lattice parameter of ~5.26 Å that would be representative of the studied temperature range of 1,073—1,173 K with IQNS.

A schematic of possible H locations in an FCC YH_x lattice with the theoretical distances between different H locations is presented in Figure 9.

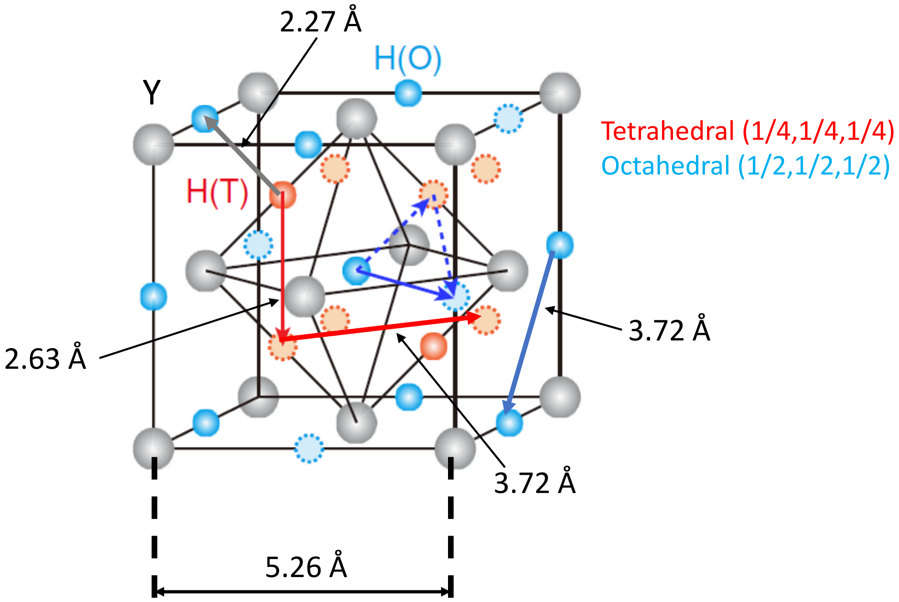


Figure 9. The FCC crystal structure, with H locations highlighted for tetrahedral and octahedral occupancy (adapted from [29]). The distances between tetrahedral and octahedral locations are also marked, as well as the lattice parameter of the $YH_{1.87}$ lattice.

At first glance, the measured average jump distance of 3.04 Å does not agree perfectly with the theoretical distances shown in Figure 9. It must be emphasized that the isotropic Chudley-Elliot model represents an average of all possible jumps in the lattice (i.e., multiple distances).

Furthermore, evidence of fast localized motion was found within the studied temperature range; the localized jump times are presented in Figure 10.

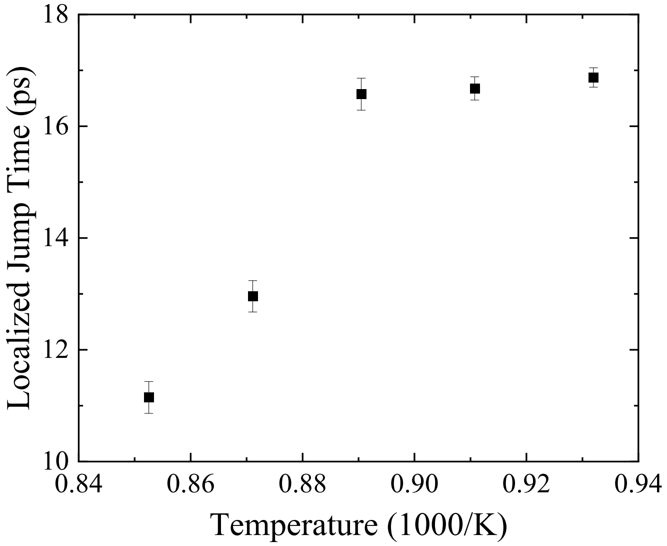


Figure 10. Localized jump times presented as a function of temperature for the sample $YH_{1.87}$.

The data from Figure 10 suggest that the H atoms are not stable in their locations within the lattice, and they frequently move away from their theoretical positions. Accordingly, the translational jump distances could be higher than their theoretically calculated values. Overall, the results suggest that the dominant jump mechanism would be between two neighboring tetrahedral locations with a theoretical distance of 2.63 Å (Figure 7). This is also the expected dominant jump mechanism at this H concentration (H/Y: 1.87), where the H atoms are expected to predominantly occupy the T sites. Finally, the high activation energy (1.76 eV) required for translational diffusivity, coupled with the absence of detectable translational motion below 1,073 K, suggests that $YH_{1.87}$ is a stable hydride at high temperatures.

Although only $YH_{1.87}$ was studied, hydrogen diffusion in yttrium hydride is also a function of hydrogen concentration, which is correlated to the available occupancy positions of hydrogen as presented earlier in this section. Most of the data available in the literature [13, 24, 30, 31] are focused on higher H concentrations for cases in which there is higher H mobility per the information presented above. To gain a more comprehensive understanding, additional IQNS experiments at BASIS, SNS, are planned to investigate hydrogen concentration dependence on hydrogen diffusion in yttrium hydride as part of the FY2021 efforts. This study on $YH_{1.87}$ provides very relevant information for the TCR design, as it specifies $YH_{1.85}$ as its moderator.

5. SUMMARY

This report presents the results of H diffusivity measurements performed on the $YH_{1.87}$ moderator material. IQNS was used to detect H motion (localized and long-range) within the temperature range of 200–1,173 K. No translational motion of H in $YH_{1.87}$ was observed for cases in which the temperature is lower than 1,073 K in the present study, as manifested by the independence of the quasi-elastic linewidth evolution on momentum transfer. For high-temperature measurements, significant evolution of the quasi-elastic line broadening as a function of momentum transfer revealed the presence of translational motion of the H atoms (i.e., diffusivity) in $YH_{1.87}$ in the temperature range of 1,073–1,173 K. The evolution of the diffusion coefficients as a function temperature was observed to follow an Arhenius-type relation. The fit to this trend revealed the activation energy (E_a) required for self-diffusion as E_a=1.73 eV. Compared to data from the literature, an E_a of 1.73eV was found to be considerably high. Coupled with the absence of translational motion below 1,073 K, the results indicate a good high temperature stability of the $YH_{1.87}$ compound.

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