INTRODUCTION

Metal hydrides such as zirconium hydride (ZrH₄) have been used as a moderator/reflector material in nuclear reactors because of their ability to retain hydrogen at elevated temperatures. Yttrium hydride (YH₂) is of interest as a potential high temperature moderator/reflector material because of its superior hydrogen density at elevated temperatures. The *ab initio* approach [1] is used to generate thermal neutron scattering laws (TSLs) for hydrogen in yttrium hydride (H-YH₂) and yttrium in yttrium hydride (Y-YH₂). The *ab initio* code VASP (Vienna ab initio Simulation Package) [2] and lattice dynamics code PHONON [3] were used to generate the dispersion relations and phonon frequency distributions for YH₂. This information was then used to prepare H-YH₂ and Y-YH₂ thermal scattering laws using the LEAPR module of the NJOY code. VASP/PHONON calculations have previously been used to generate TSL data for Be [1], high density graphite [1,4], ThH₂ [5], α-SiO₂ [6], and were used to prepare the ENDF/B-VII.1 TSL evaluation for α-SiO₂ [7].

CRYSTAL STRUCTURE AND LATTICE DYNAMICS

YH₂ has a CaF₂ type face-center cubic (FCC) structure. The unit cell is composed of 12 atoms with the hydrogen atoms located in the tetrahedral holes between the Y atoms. The structure of the YH₂ unit cell is shown in Fig. 1 with the Y atoms colored blue and the H atoms colored light grey. As optimized by VASP, this structure has a lattice constant of a = 5.2032 Å, which agrees with the average experimental value of a = 5.204 Å [8].

The VASP code performed first principles quantum mechanics simulations of the YH₂ lattice structure using density functional theory with a generalized gradient approximation (GGA) and a projector augmented wave (PAW) pseudopotential. The YH₂ lattice structure was optimized to a total energy threshold of 0.0001 eV using the MedeA automated convergence tool [9]. The dispersion relations and density of state were calculated using the MedeA-PHONON tool. A 2×2×2 supercell (96 atoms) with a 250 eV planewave cutoff energy was used to calculate the dispersion relations. The phonon frequency distribution (density of states) was calculated using a ± 0.02 Å displacement.

Fig. 2 shows the dispersion relations along the highest symmetry points of the Brillouin zone derived from the PHONON calculation. The lower branches are acoustical modes which are mainly due to the heavy Y atom vibrations. The higher branches are optical modes mainly due to the H atom vibrations.

[Diagram showing dispersion relations]

**Fig. 2. Ab initio calculated YH₂ dispersion relations**

Fig. 3 shows the partial phonon frequency distributions calculated for YH₂. The phonon density of states has two well-separated regions (due to the large
mass ratio between Y and H): an acoustical region (0-0.027 eV) which is the preferred region for Y atom vibrations and an optical region (0.110-0.140 eV) which is the preferred region for H atom vibrations. The optical region is centered at ~0.125 eV which compares well with the 0.128±0.004 eV estimate by Flotow [10] derived from heat capacity measurements and the 0.127±0.007 eV value recommended by Rush [11] derived from neutron scattering measurements. The YH₂ optical mode in more recent neutron scattering measurements by Udovic [12] displayed a similar bimodal structure centered at ~0.125 eV.

Thermodynamic properties of YH₂ can also be calculated from the phonon density of states. Fig. 4 show the calculated heat capacity for YH₂ which compare well with measurements by Flotow [10].

ENDF/B-VII.1 atomic mass ratio and free atoms scattering cross section data for ¹H and ⁵⁷⁷Y were used to develop the TSLs. The α and β mesh were borrowed from the ENDF/B-VII.0 H-ZrH and Zr-ZrH evaluations. TSLs were generated at 10 temperatures: 293.6, 400, 500, 600, 700, 800, 1000, 1200, 1400 and 1600 K. Fig. 5 shows the inelastic scattering and incoherent elastic scattering cross sections for H-YH₂. The inelastic scattering and incoherent elastic scattering cross sections for Y-YH₂ given in Fig. 6.

**THERMAL SCATTERING LAWS**

TSLs for H-YH₂ and Y-YH₂ were developed from the phonon frequency distributions calculated by MedeA-PHONON using the LEAPR module of NJOY [13].
CONCLUSIONS

Computational material science tools such as VASP and PHONON appear to have matured to the point where they can be used to calculate TSLs for new moderator materials of interest in nuclear applications. TSLs for H-YH₂ and Y-YH₂ have been generated using the ab initio approach and compare well to the limited available measurements. Cross section measurements are needed to validate the YH₂ TSL evaluations.

REFERENCES