Physics-Based Uncertainty Quantification for the ZrH_x Thermal Scattering Law

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INTRODUCTION

In TRIGA reactors, such as the Texas A&M Nuclear Science Center, U-ZrH_x is used as the fuel material. At thermal energies, the neutron scattering from ZrH_x is heavily affected by the frequency distributions, also called *phonon spectra*, associated with the solid structures.

Currently, the phonon spectrum models of the bound system of ZrH_x used to generate thermal scattering data in ENDF were developed by Slaggie by using central force (CF) model in GASKET (1967) [1]. Malik et al. derived a multi-Gaussian model for the optical part of the frequency distribution of H based on experimental results[2]. New evaluations, which are said to have better agreement with experiments, were done by Mattes et al. [3]. Mattes et al. derived a Debye-plus-Gaussian (DG) phenominalogical model for H binding and treats the Zr as free gas in the molecule. All these articles are based on the molecule has fixed phonon states despite the fact that actual fuel is a mixture of several types of zirconium hydride in different phases, the phonon spectrum must be different from the one from CF or DG models[4, 5].

Nevertheless, the DG model has benefit of agreeing well with experiments despite its simple form consisting of Debye and Gaussian distributions. These facts inspired us to develop a similar simple parameterized mathematical model for the H part of the spectrum and use simple parameterized curves that have similar shapes with the Zr spectrum in CF model to represent our model for Zr in ZrH_x.

In this work we have established parameterized phonon spectrum models for H and Zr in ZrH_x to account for the uncertainty of the spectrum due to the uncertainty of the solid structure. The quantitive relationships between quantities of interests (QOIs), which currently include reactivity and fission rate density (FRD) for a TRIGA lattice model, and the parameters are established. Our model and results also allow us to determine parameters have the largest effect on QOIs.

THEORY AND ALGORITHMS

In the bound system of ZrH_x, two types of scatterings are concerned at the thermal energies: they are incoherent inelastic scattering and coherent elastic scattering. Coherent scattering, an important phenomenon in crystalline solids (e.g., graphite) but not in hydrogenous solids ZrH_x[6], is not included in this study. One aim is to build the thermal scattering law for the incoherent inelastic scattering and simultaneously calculate the Debye-Waller integral such that we can calculate the incoherent elastic scattering cross sections.

It is assumed that the scatterings, including inelastic and elastic, are azimuthally isotropic. With this assumption, the angular scattering cross sections are with per steradian.Then the double differential scattering cross section (DDXCS) can be written as:

$$\sigma(E'\to E, \mathbf{\Omega}\cdot\mathbf{\Omega}) = \frac{\sigma_b}{4\pi kT}\sqrt{\frac{E}{E'}}S(\alpha,\beta), \tag{1}$$

where E' and E are the incident and secondary neutron energies. The $S(\alpha,\beta)$ is called thermal scattering law. The definitions of α and β are:

$$\alpha \equiv \frac{E+E'-2\mu\sqrt{EE'}}{AkT} \text{ and } \beta \equiv \frac{E-E'}{kT} \tag{2}$$

α and β are the momentum and energy transfer, respectively. A is the ratio of scatterer mass to neutron mass. With the Gaussian approximation[7] the scattering law can be expressed as:

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\beta t}e^{-\gamma(t)}dt \tag{3}$$

where t is a non-dimension time which is measured in the units of $\hbar/kT$. $\gamma(t)$ is given by

$$\gamma(t) = \alpha\int_{-\infty}^{\infty}\frac{\rho(\beta)}{2\beta\sinh(\beta/2)}[1-e^{-i\beta t}]e^{-\beta/2}d\beta \tag{4}$$

where $\rho(\beta)$ is the phonon spectrum of the bound system. It contains all the information we need to compute the scattering law. Therefore, specifying a phonon spectrum is, in some sense, equivalent to specifying a scattering law.

Phonon spectra used to tabulate scattering laws of Zr and H of ZrH_x in ENDF-VII were generated with Slaggie's central force model[1, 6]. More recently, Mattes et al. [3] used a simplified spectrum developed by Slaggie[1] for H and treated Zr as free gas. The model is a Debye-plus-Gaussian-phenomenological (DG) model and we refer to it as the IKE model. It contains an acoustic part which has a Debye temperature of 20meV and an optical part which is an Gaussian distribution with a mean of 137meV and an FWHM of 28meV[1].

We have developed a new model for the H-H binding such that it is parameterized and developed an adjustable model for Zr-Zr binding. For H, the spectrum can be given by

$$\rho(\omega)_{\mathrm{H}} = \begin{cases} \frac{3b}{2T_{\mathrm{DH}}^3}\omega^2 & \omega < T_{\mathrm{DH}} \\ \frac{3b}{2T_{\mathrm{DH}}^3}(\omega-2T_{\mathrm{DH}})^2 & T_{\mathrm{DH}} \le \omega \le 2T_{\mathrm{DH}} \\ \frac{g(b)}{\sqrt{2\pi}\sigma}\exp\left[-\frac{(\omega-p)^2}{2\sigma^2}\right] & 2T_{\mathrm{DH}} \le \omega \le \omega_{\max,\mathrm{H}}. \end{cases} \tag{5}$$

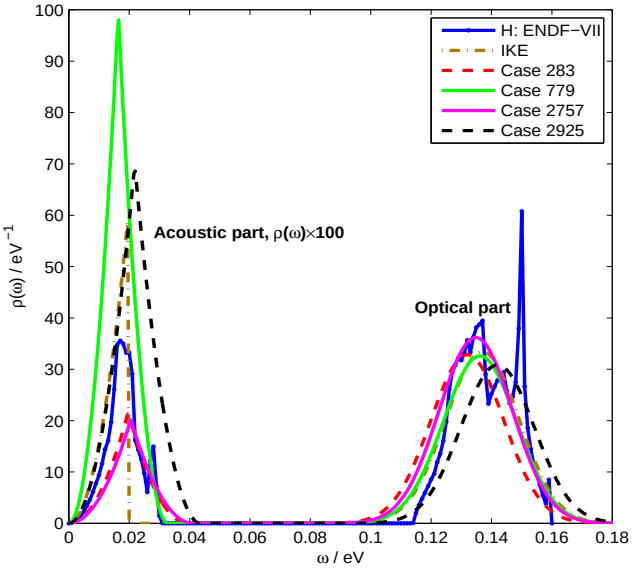

Fig. 1. The reference spectrra and four Examples of the paramterized model of H in ZrH_x.

For Zr, the spectrum is given by

$$\rho(\omega)_{\mathrm{Zr}} = \begin{cases} \frac{r(1+c)}{T_{\mathrm{DZr}}^{1+c}}\omega^c & \omega < T_{\mathrm{DZr}} \\ \frac{(1+c)r}{T_{\mathrm{DZr}}} \exp\left[\frac{(1+c)^r}{1-r}(1-\frac{\omega}{T_{\mathrm{DZr}}})\right] & T_{\mathrm{DZr}} \le \omega \le \omega_{\mathrm{max,Zr}}. \end{cases} \tag{6}$$

Note that

$$\int_0^\infty \rho(\omega)d\omega = \int_0^\infty \rho(\beta)d\beta \text{ and } \beta = \frac{E-E'}{kT} = \frac{\omega}{kT}, \tag{7}$$

where ω is in units of eV.

In Eq. 5 , b is the branching ratio of the acoustic part; T_{DH} is the Debye temperature of H in ZrH_x; p is the peak position of optical peak; σ, calculated from the $FWHM$ of the optical part, is the standard deviation of the Gaussian distribution; the $g(b)$ is a function of b and the normalization coefficient and $g(b) \approx 1 - b$. In Eq. 6, T_{DZr} is the peak position of the spectrum; c is the power of ω for the left side of peak; r is the ratio of the left part of the peak to the whole spectrum. In total, our parameterized spectra has seven parameters: b, T_{DH}, p, $FWHM$, T_{DZr}, c and r. Figure 1 contains some examples of the parameterized model of the H part compared with the ENDF-VII and IKE models with different combinations of parameters, which lead to different spectra shapes from a Latin Hypercube sampling.

Code to Code Comparison

We have developed a code to calculate the scattering data, e.g. DDXCS and $\sigma(E' \to E)$ of ZrH_x based on the model, the theory and algorithms above. One aim of the work is to calculate the cross sections and investigate the impact of a parameterized model on the scattering data by varying the seven input parameters. Comparisons were performed by using the THERMR module in NJOY[8] and our code with some common set of parameters. Quantities like $\sigma(E' \to E)$, $\bar{\mu}$, etc., were calculated. Our model demonstrated good agreement with the NJOY calculations.

IMPACT OF THE PARAMETERIZED MODEL OF THE BOUND SYSTEM ON TRIGA REACTOR LATTICE

Another aim is to model the effects of the parameterized model on QOIs, i.e. reactivity and FRD. NJOY and MCNP were used to do the calculations an infinite lattice of TRIGA pins. The calculation procedure was:

1. Given ranges of all seven parameters, use the Latin Hypercube Sampling method (LHS)[9] to sample 3000 sets of parameters; all the parameters are uniformly distributed;
2. With the parameters generated in LHS, generate the phonon spectra for H-H binding and Zr-Zr binding;
3. The LEAPR, THERMR, ACER and VIEWR modules in NJOY are invoked to generate and check the data with which MCNP is compatible;
4. Use MCNP to do the criticality calculations for the TRIGA lattice with all the generated data files;
5. Analyze the criticality calculation results.

Modeling and Analyses

The two QOIs were extracted from MCNP output files. We built a regression model of the results for each QOI. For feature selection we investigated models all 7 main effects from each parameter and all 21 pairwise interactions between parameters. Our final model had all 7 main effects and 5 interaction terms. Cross-validation tests, shown in Fig. 2, confirm the efficacy of this model. Based on the statistical model for ρ we found that b (the branching ratio for H) and p (the optical peak position in H) are the main factors affecting reactivity. N-way ANOVA analyses indicate similar conclusions. However, FRD is found to be insensitive to any of these parameters. It behaves like random noise around a constant for this particular problem.

Two more cases with ENDF-VII and IKE thermal scattering law data were run and results were plotted with those from the parameterized model using a scatterplot within the plane of the two QOIs as shown in Fig. 3. It is observed that these reference results are within the range generated by our model.

CONCLUSIONS

This work develops parameterized models of phonon spectra for H and Zr in ZrH_x, respectively, with seven parameters assumed. And a code based on the model has been developed to calculate the scattering data like DDXCS and group constants, etc. Comparisons between the code and NJOY has been taken and results from the code agree to NJOY's results

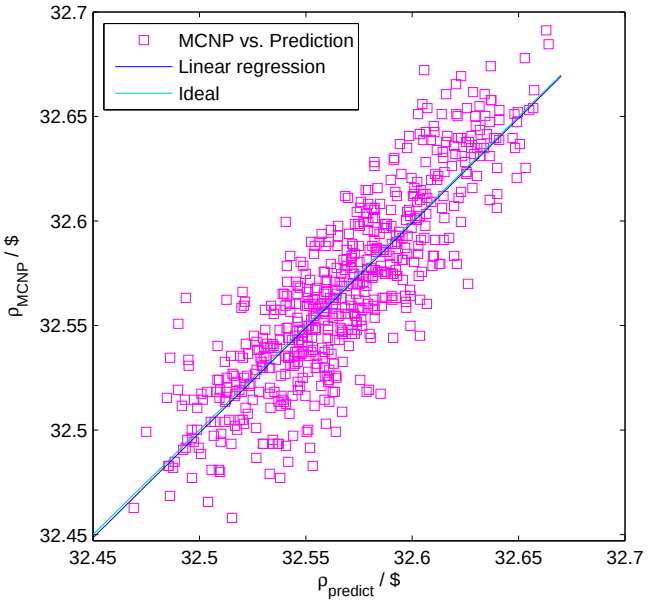

Fig. 2. Cross-validation test of the statistical model of ρ versus the actual MCNP result for the testing data. For the regression, $R^2 = 0.7341$and $RMS\,E_\rho = 0.0250$.

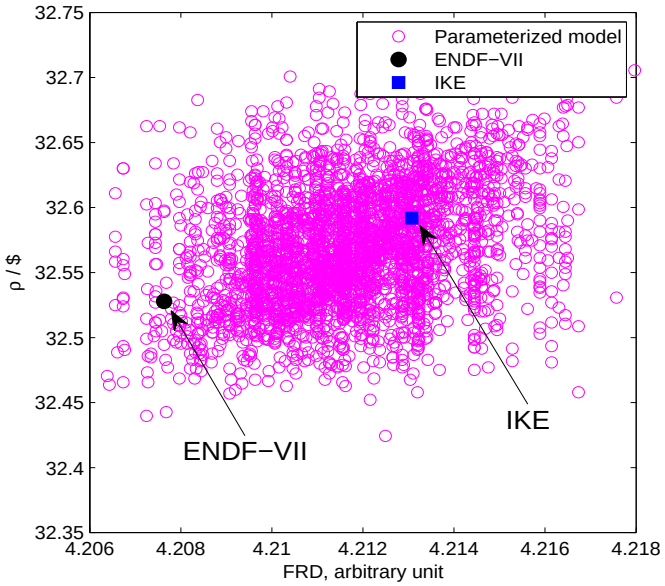

Fig. 3. Comparison between references and the parameterized model.

for some common set of parameters. We investigated the effects of the parameters in our model on reactivity and FRD in a lattice of ZrH_x pins. Based on a statistical model of our results the main factors driving reactivity are the branching ratio and the optical peak in the phonon spectrum for H.

In the future we plan to apply our results, namely the important parameters in the ZrH_x model, full-core simulations of TRIGA reactors, including coupled thermal hydraulics/neutronics simulations of pulses. An intermediate step will investigate the effects of the two main parameters on the full-core neutronics simulations.

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