On the impact of phonon spectrum shifts of the hydrogen binding in ZrH

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Goal: the accurate evaluation of the reactivity feedback in TRIGA cores within the ECATS project (Experiment on a Coupling of an Accelerator, a spallation Target and a Subcritical blanket) to study dynamic feedbacks in Source-Driven Sub-critical systems.

Introduction

* The standard reactivity feedback curve (GA-General Atomic) differs from new experimental data, in particular in range of 80-140^{O} Celsius;

* The influence of the numerical treatment with respect to the preparation of scattering kernel S(α,β) for the hydrogen bound in zirconium hydride , on the negative reactivity coefficients is analysed;

* The impact of the inter-molecular forces in form of the phonon distribution function and of a shifted phonon peak on the energy scale on the reactivity coefficients is introduced;

Model: description and input

TRIGA fuel assembly model

* Fuel elements are cylinders of ternary alloy uranium zirconium hydride with H-to-Zr ratio 1.7 and total Uranium of 8,5% of the mixture by weight and 20% enriched U -235

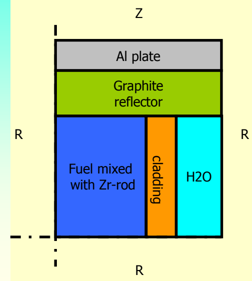
* Fuel cladding – stainless steel AISI 304

* Two graphite cylinders at the top and the bottom of the fuel rod

* Two aluminum plates at the top and the bottom of the fuel rod

R – reflective boundary condition

Z – zero flux boundary condition



Experimental Results

* The reactivity measurements were carried out in two similar TRIGA cores:
- TRIGA RC-1 Casaccia, Italia with burned-up fuel – since 1967 -115FA
- TRIGA Mark II Ljubjana, Slovenia with fresh fuel – 47.6 FA

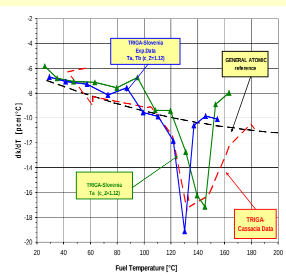
* In both experiments only one or two temperature measurement points were applied from which an average temperature was evaluated by the formula used in the Benchmark paper

* All curves differ considerably from the General Atomic (GA) curve in range (110-150 Celsius degree)

a) The two curves of the Slovenian core are based on two point measurements at the centre of the core (A -Ta) and at the first ring of the core (B-Tb)

b) The Cassacia curve was taken from TRADE report

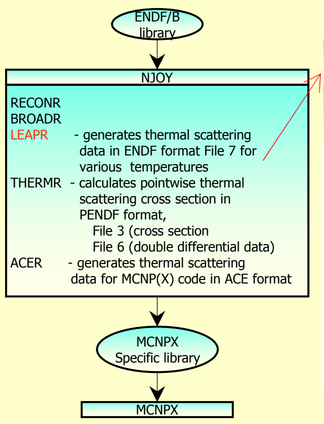
* The differences between the curves emphasizes the necessity of a multi-point temperature measurement to asses more accurately the influence of the spatial flux distribution and the fuel content on the reactivity feedback.



Experimental temperature dependent reactivity feedbacks of the Cassacia and Slovenian TRIGA cores

TRIGA RC-1 Cassacia

Cross section and scattering kernels processing



Phonon expansion method

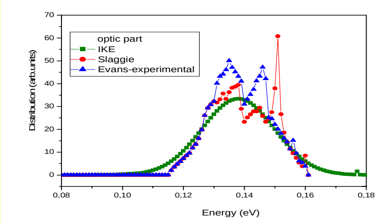
Approximation for bound isotopes in molecules (Slaggie and IKE)

$$S_S(\alpha,\beta) = e^{-\alpha\lambda_S} \sum_{n=0}^{\infty} \frac{1}{n!}\alpha^n x \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta\hat{t}} [P_S(\beta')e^{-\beta'/2} e^{-i\beta'\hat{t}} d\beta]^n d\hat{t}$$

is the thermal scattering law

α is the momentum transfer, β is the energy transfer

ρ(β) is frequency spectrum, and λ is the Debye-Waller coefficient



Investigated and experimental frequency distribution of hydrogen bound in zirconium hydride

Sensitive issues for Light Isotopes

a) Face centered cubic (fcc) structure

b) Phonon frequency distribution (LEAPR)

c) Choice of energy grid in THERMR (old standard 59 points, new 118)

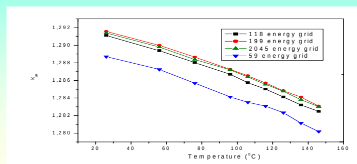
d) Equi-probable energy interval points in ACER

e) Number of Cosine bins in THERMR

f) Tolerance for cross section reconstruction in RECONR and BROADR

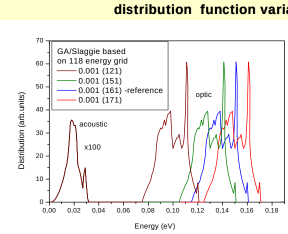
g) Free gas kernel for secondary scatterer

MCNPX 2.5d calculated criticality values using different S(α,β) input files for hydrogen bound in zirconium

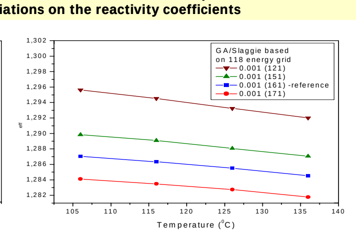


Case c)

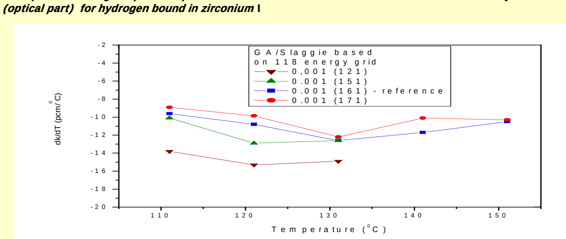
The influence of the intermolecular forces in form of the phonon distribution function variations on the reactivity coefficients



*Examples of shifting the phonon spectrum (optical part) for hydrogen bound in zirconium *



MCNPX 2.5d calculated criticality values



The impact of different phonon spectrum (optical part) in the reactivity feedback

Conclusions and Summary

* The improved energy grid scheme in the NJOY update 112 for module THERMR is not completely adequate and about 80 more points seems to be needed for hydrogen bound in zirconium;

* The changes of the phonon spectrum itself in the temperature range 100-140 Celsius degree could explain the specific behavior of the temperature dependent reactivity coefficient in the TRIGA subassembly;

* An experimental based physical confirmation is needed, including also detailed measurements of hydrogen bound in fuel matrix with zirconium;

* The stoichiometry and the intermolecular forces have mainly influence on the criticality and they should merged together with spectrum effect;

* The resulting improved model for the ZrH – scattering kernel is of high interest if TRIGA reactors will be applied for fundamental neutron physics experiments, as e.g. proposed in the ECATS program of EC integrated project EUROTRANS;

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