National Key Laboratory of Intense Pulsed Radiation Simulation and Effect

Neutronic Properties of Metal Hydride Moderators and Their Applications in Microreactors

Lipeng Wang

Northwest Institute of Nuclear Technology

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1、Application of metal hydride moderator in micro-reactor

- Microreactors have demonstrated significant application potential across land, sea, air, and space domains –owing to their compactness, inherent safety, and modular design advantages.

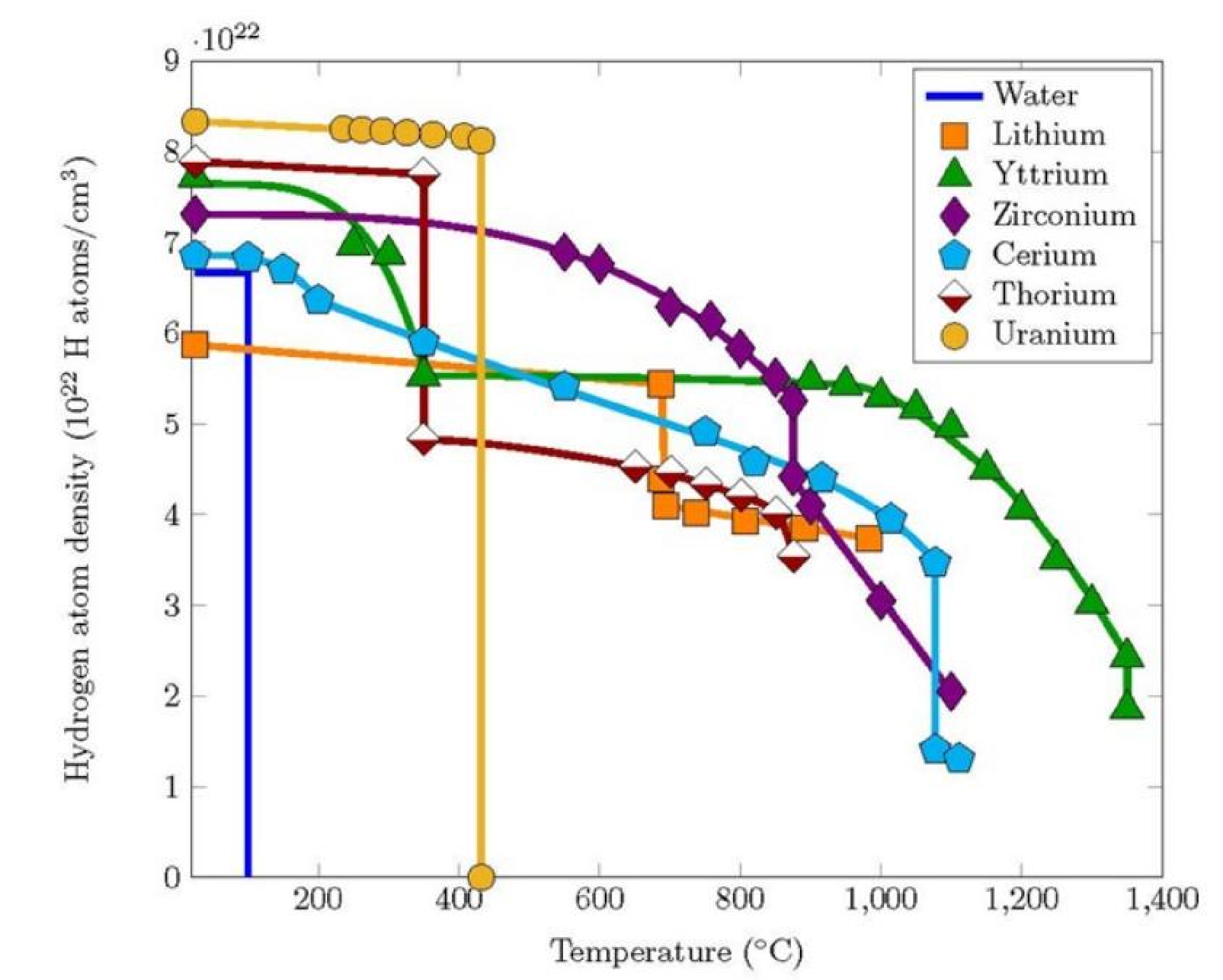
- Given the mobile nature of most microreactors, solid moderators become essential to minimize moderator system volume and mass, reduce fuel enrichment requirements, and ensure operational safety.

- Metal hydrides serve as effective solid moderators, exhibiting hydrogen atomic concentrations significantly exceeding those of liquid hydrogen counterparts. This characteristic makes metal hydride moderators particularly suitable for thermal reactors requiring minimized core weight and volume.

1、Application of metal hydride moderator in micro-reactor

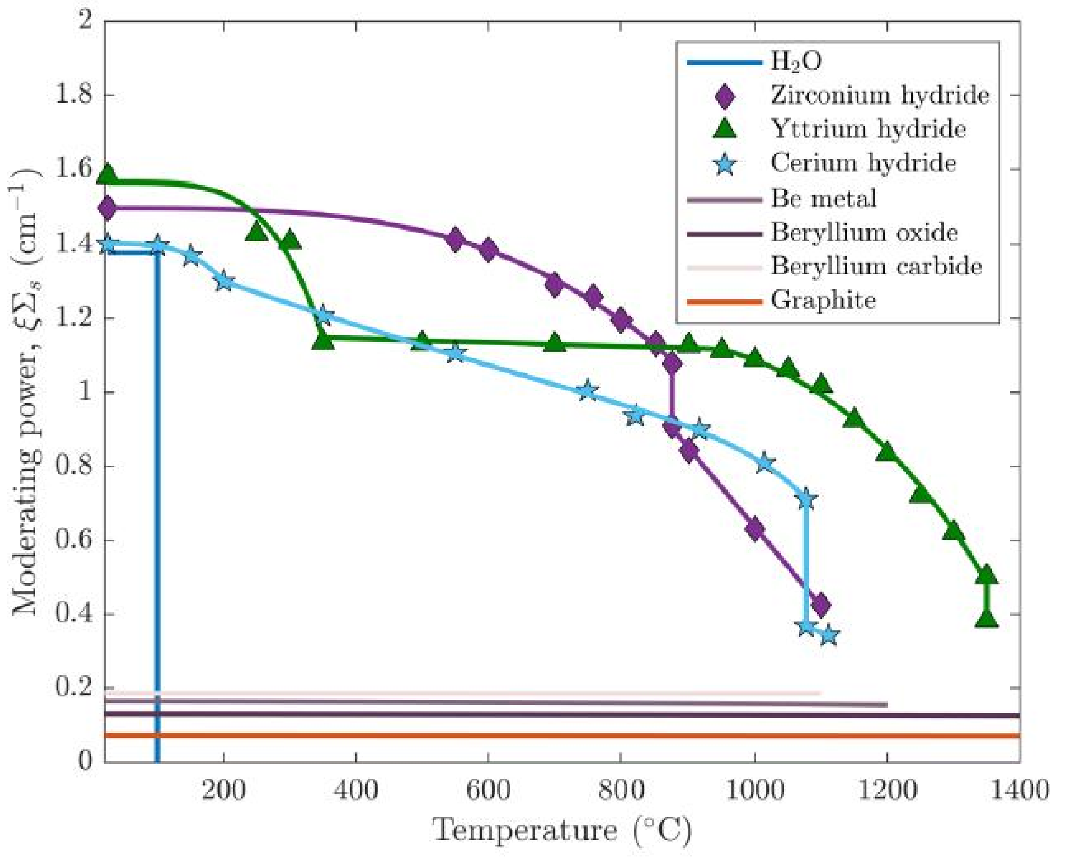
➢ **Figure 1 illustrates the hydrogen content of various metal hydrides at different temperatures. It can be observed that when temperatures exceed 700° C and 850° C, the hydrogen atomic density in lithium hydride (LiH) and zirconium hydride (ZrHx) decreases rapidly. In contrast, yttrium hydride (YHx) maintains a significantly higher hydrogen atomic density even at 1000° C or above. Owing to its superior hydrogen density (>150×10²² atoms/cm³) and high-temperature stability (>800° C), yttrium hydride is recognized as an ideal moderator for microreactors and has been implemented in multiple reactor designs.**

Metal hydride	10^{22}H atoms H/cm³	g H/cm³	g/cm³	Moderator ability	Moderator ratio
TiH_2	9.1	0.152	3.78	1.85	6.3
ZrH_2	7.3	0.122	5.56	1.45	55
LiH	5.8	0.095	0.78	1.2	3.5
YH_2	5.8	0.097	4.24	1.2	25
ThH_2	4.9	0.082	9.5	1.0	5.2



1、Application of metal hydride moderator in micro-reactor

- Figure 2 displays the temperature-dependent moderating power of various conventional moderator materials. It is observed that water and metal hydrides exhibit significantly higher moderating power compared to beryllium compounds and graphite, as their primary moderating nuclei are hydrogen atoms, which more efficiently thermalize neutrons. However, a key advantage of beryllium-containing compounds and graphite lies in their near-constant moderating power across temperatures, with only minor variations attributable to thermal expansion.
- In contrast, metal hydrides demonstrate a gradual decline in moderating power with rising temperatures, driven by temperature-dependent equilibrium hydrogen content. Yttrium hydride (YHx) emerges as an attractive metal hydride moderator, as its hydrogen content remains relatively stable in pure hydrogen at 1 atm, whereas zirconium hydride (ZrH2) and cerium hydride (CeH3) suffer hydrogen loss under similar thermal conditions. Notably, yttrium hydride retains superior moderating capabilities even above 1000° C, making it uniquely suited for high-temperature microreactor applications.



1、Application of metal hydride moderator in micro-reactor

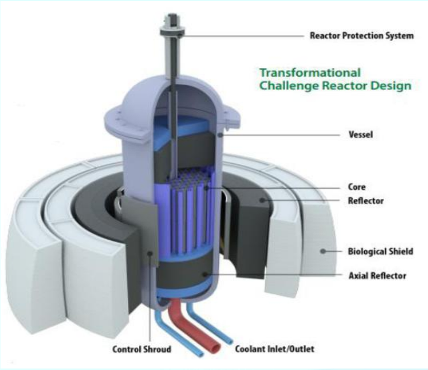
Metal hydrides serve as highly effective solid moderators, characterized by their superior hydrogen atomic concentration which far exceeds that of liquid hydrogen itself, making them an ideal choice for solid moderation. Since the 1950s–1960s, metal hydrides have been progressively implemented in reactor moderator materials, including:

- **Integrated fuel-moderator systems: TRIGA-type research reactors, the SNAP series reactors for space nuclear power exploration, and the MARVEL microreactor demonstration;**
- **Separated fuel-moderator configurations: TOPAZ series reactors, pebble-bed reactors (PBR), 3D-printed TCR reactors, and the EMPIRE reactor.**

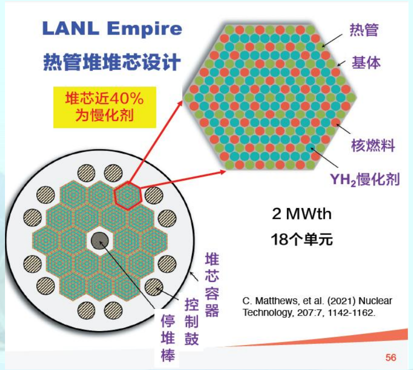
Key application domains encompass research reactors, space exploration missions, and mobile vehicular reactor power systems, highlighting their extensive potential across advanced nuclear technologies.

TRIGA、SNAP and MARVEL

TOPAZ II（ZrHx）



TCR（YHx）



Empire（YHx）

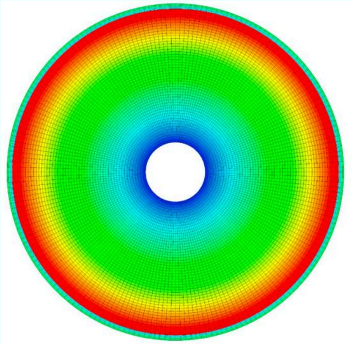
1、Application of metal hydride moderator in micro-reactor

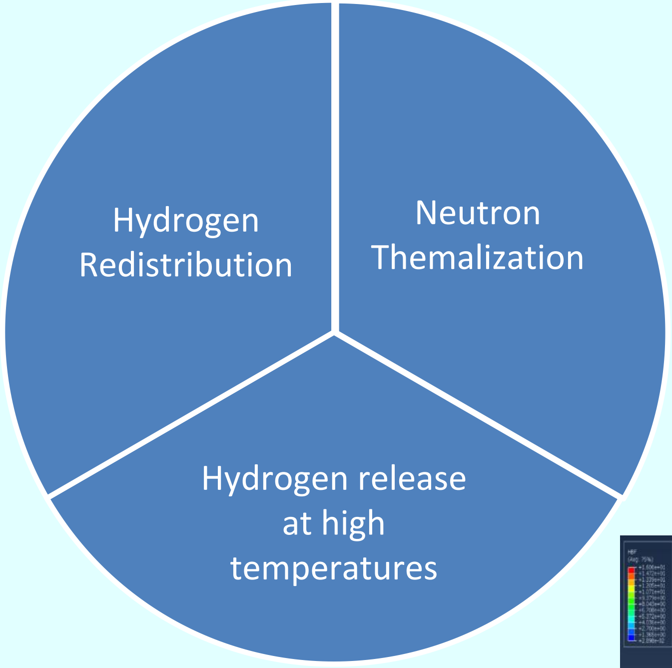
To address nuclear safety concerns associated with metal hydrides in microreactor design and applications, this study focuses on :

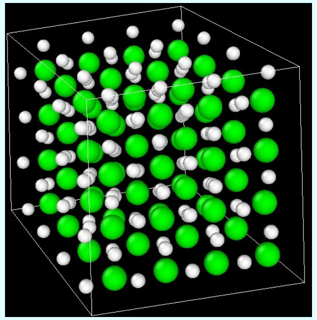
1.Ambiguity in thermalization mechanisms – Elucidating neutron thermalization dynamics in metal hydride lattices;

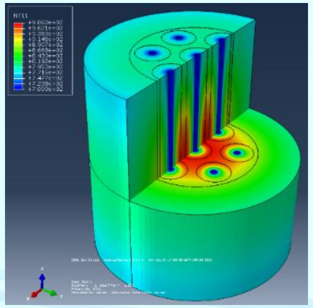
2.Hydrogen release at high temp– Evaluating how the hydrogen release phenomena reveal

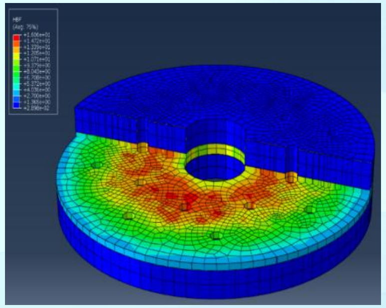
3.Incomplete understanding of hydrogen redistribution – Mapping hydrogen migration behavior .











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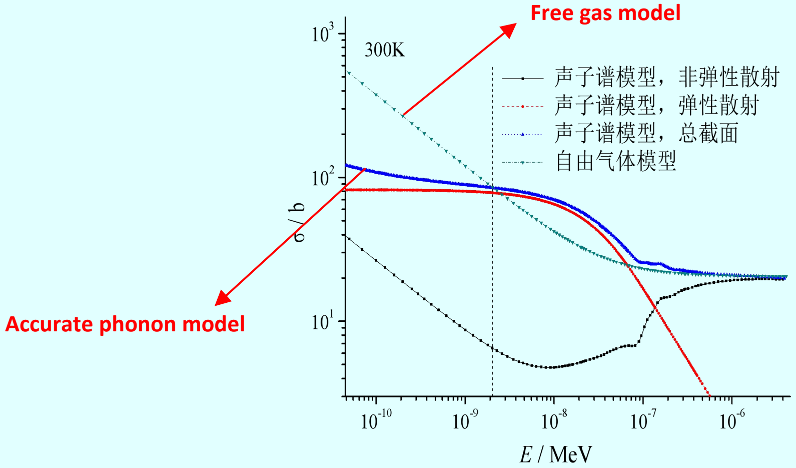
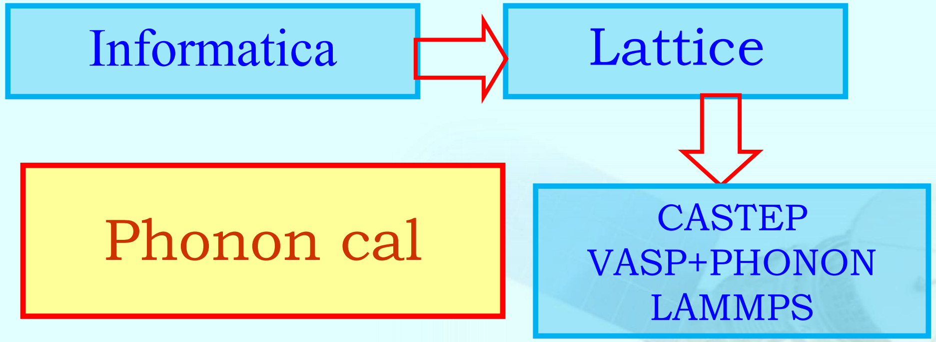
2、 Neutron Themalization

❖ Neutron thermalization mechanism of micro-reactor moderator

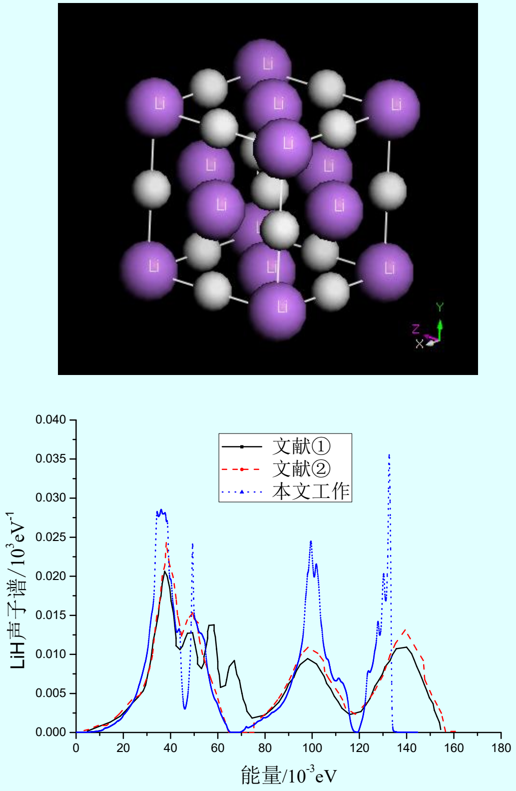
- The temperature effect of conventional metal hydride moderator is usually treated by free gas and semi-empirical phonon model. It is difficult to apply to the reactor which is sensitive to the neutron thermal effect of moderator.
- Due to the influence of the core layout and the metal hydride moderator, the temperature effect of the moderator may be positive, which seriously affects the safety performance of the reactor.
- Study on Generic Thermal Neutron xs Production and Treatment Method Based on First Principle



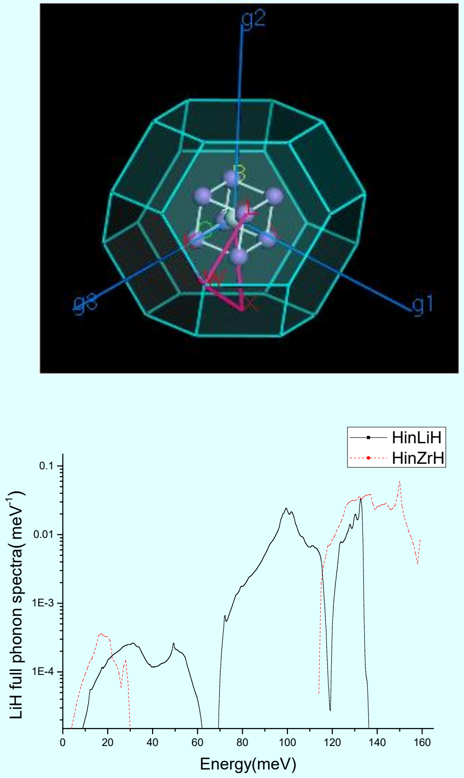


2、 Neutron Themalization

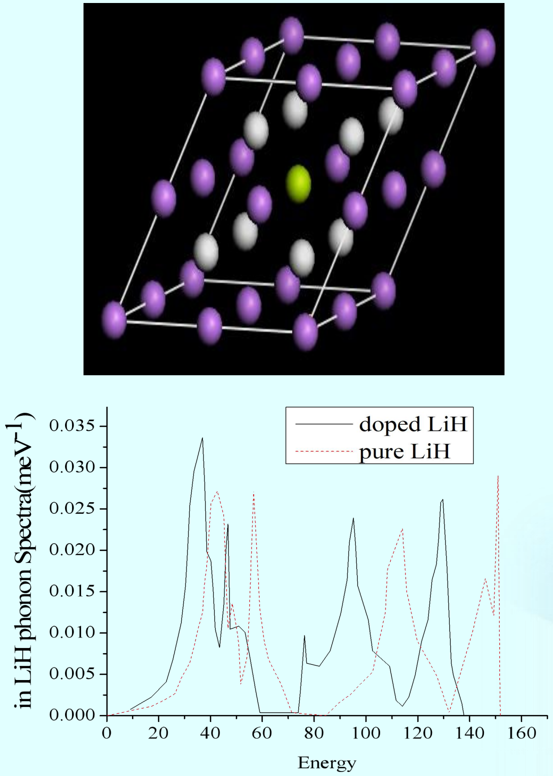
➢the phonon density of LiH,ZrHx and YHx have been studied.



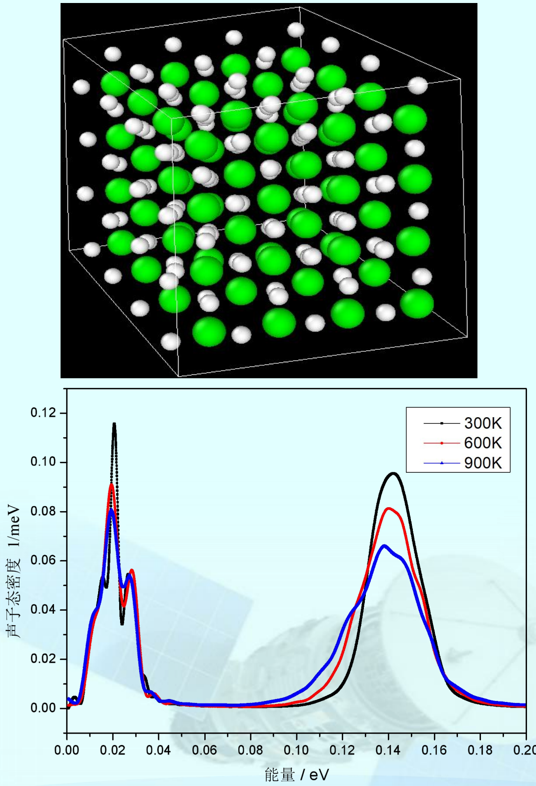
LiH phonon



H in LiH and ZrHx



Doped LiH

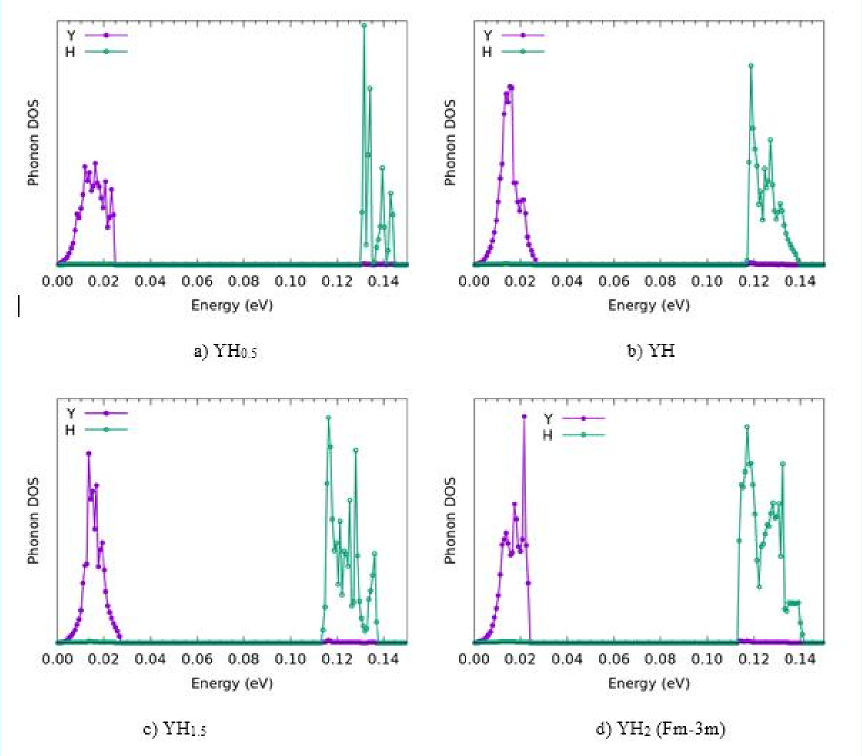


Different temp’s ZrHx phonon

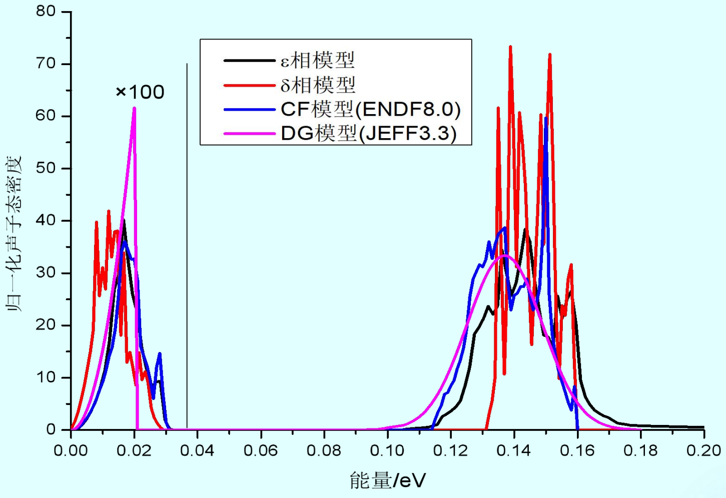
第一性原理分子动力学

2、 Neutron Themalization

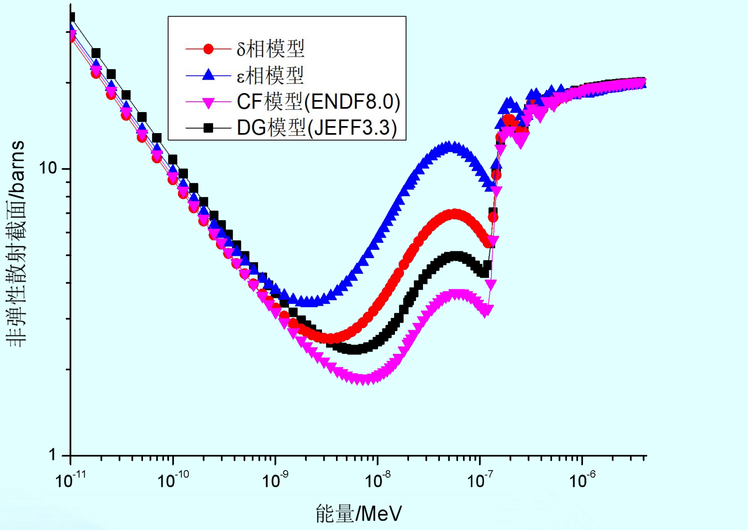
- The phonon state density of metal hydride with different ratio of elements and phase structure was compared and analyzed



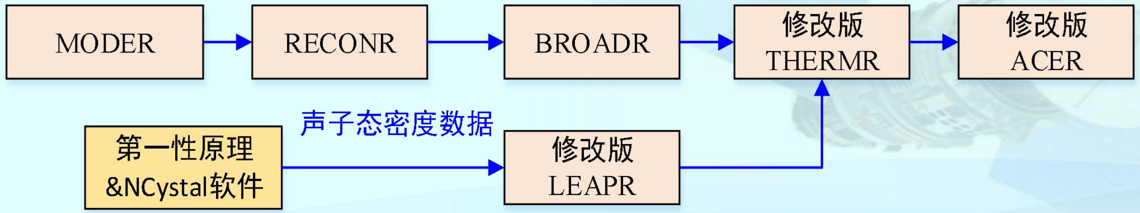
Different H/Y phonon



Different phase ZrHx phonon



Different phase ZrHx thermal neutron XS



NJOY+NCrystal Flow

2、 Neutron Themalization

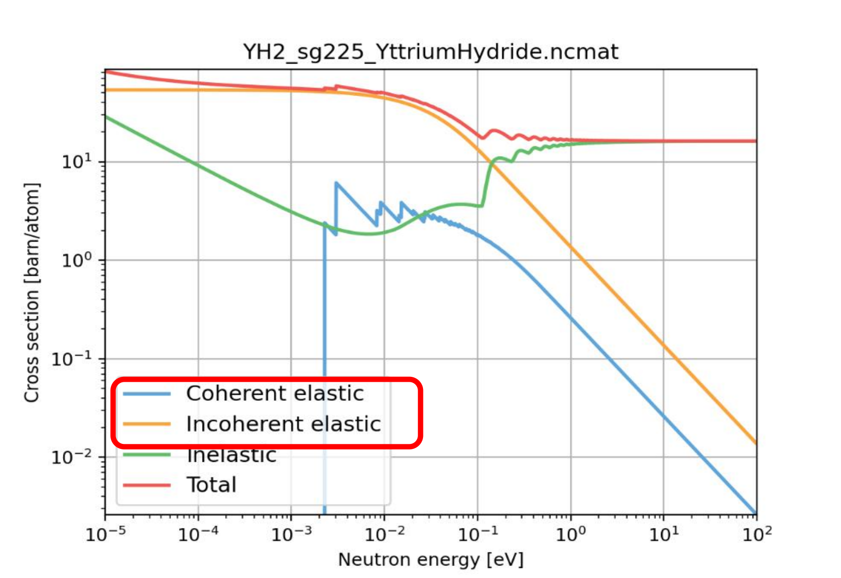
❖ Mixed elastic xs and Adaptive energy grid

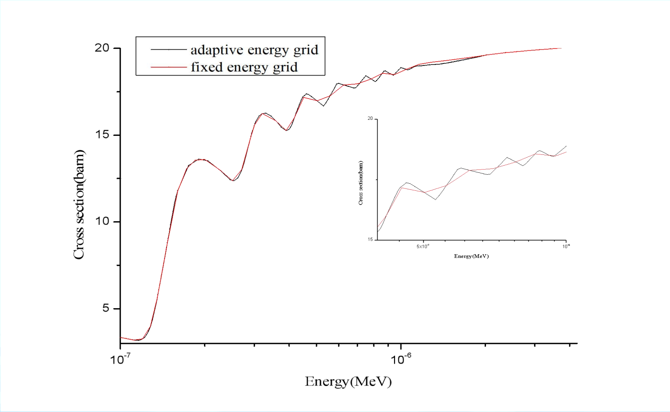
For metal hydride, we can consider both elastic and inelastic part for H and metal, whereas NJOY can only choose one.

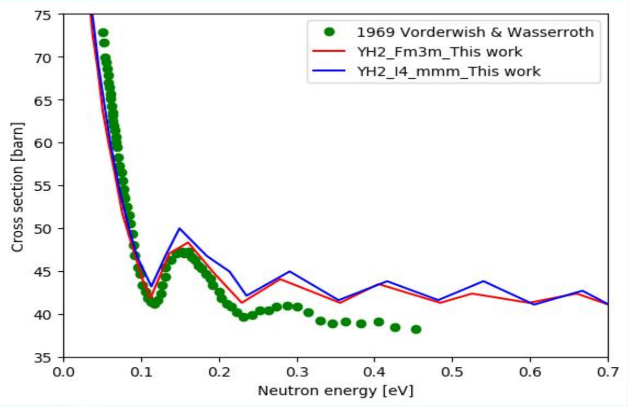
For the oscillation of the inelastic cross section of metal hydride, how to provide a suitable energy grid related to material is the key to accurately generate the inelastic cross section in the next step.

The purpose of the adaptive method is to embed physical data in S data to provide high fidelity cross section data.

Lattices → Phonon → S(alpha, beta) → TSL xs





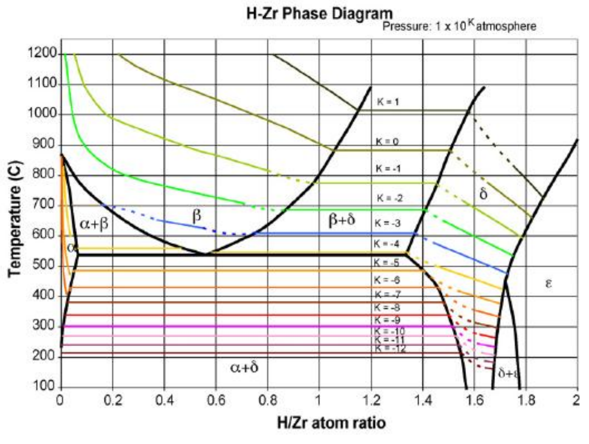


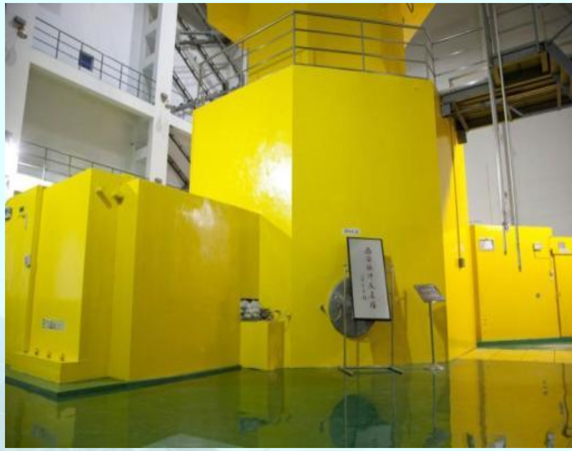
2、 Neutron Themalization

❖ Thermal kernel effect

➢ the ZrH1.6 thermal data of the precise phonon model is used to solve the problem of transient supercritical safety evaluation under the transient condition of the XAPR pulse reactor. The influence rule of transient supercritical safety parameters of XAPR is precisely mastered.

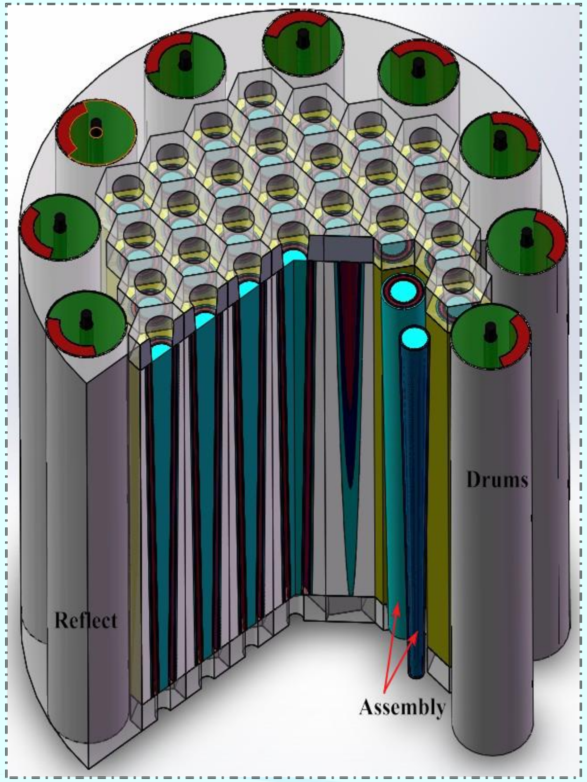
ZrHx Phonon	k_{eff} (H/Zr=1.6,300K)	k_{eff} (H/Zr=1.6,800K)	Coefficient (pcm/K)
CF(ENDF8.0)	1.011610	0.972446	-13.055
DG(JEFF3.3)	1.012553	0.973134	-13.140
δ model	1.009277	0.972164	-12.371
ε model	1.005113	0.971179	-11.311
Max difference	744 pcm	196 pcm	1.829 pcm/K



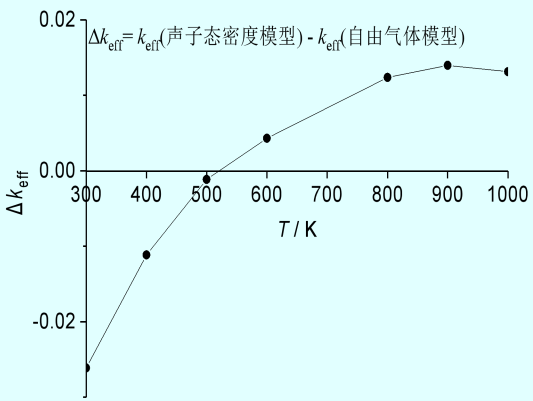


2、 Neutron Themalization

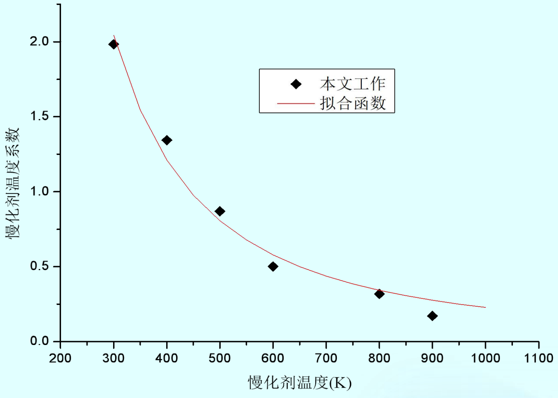
➢ *A comparative analysis of PBR criticality safety characteristics under different phonon models was conducted, revealing generalized trends in the moderator temperature reactivity coefficient (MTC)。*



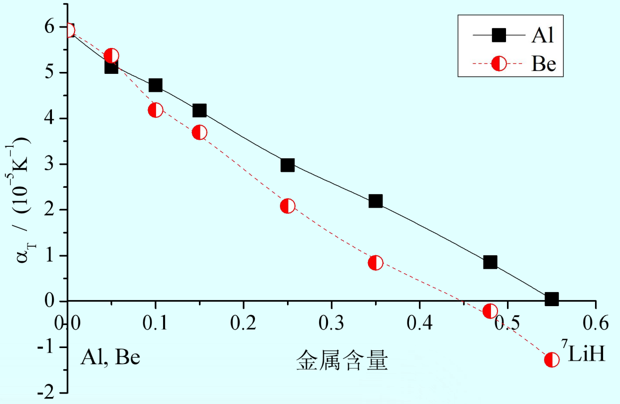
PBR(LiH moderating)



Comparison with free gas model



MTC with temp



Doped LiH MTC

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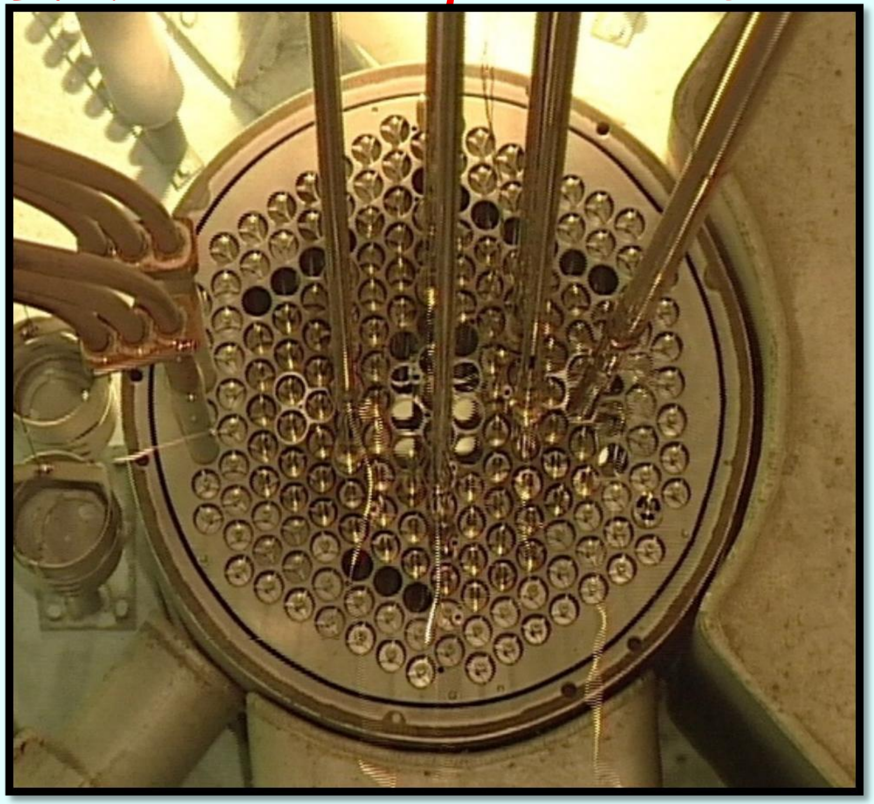
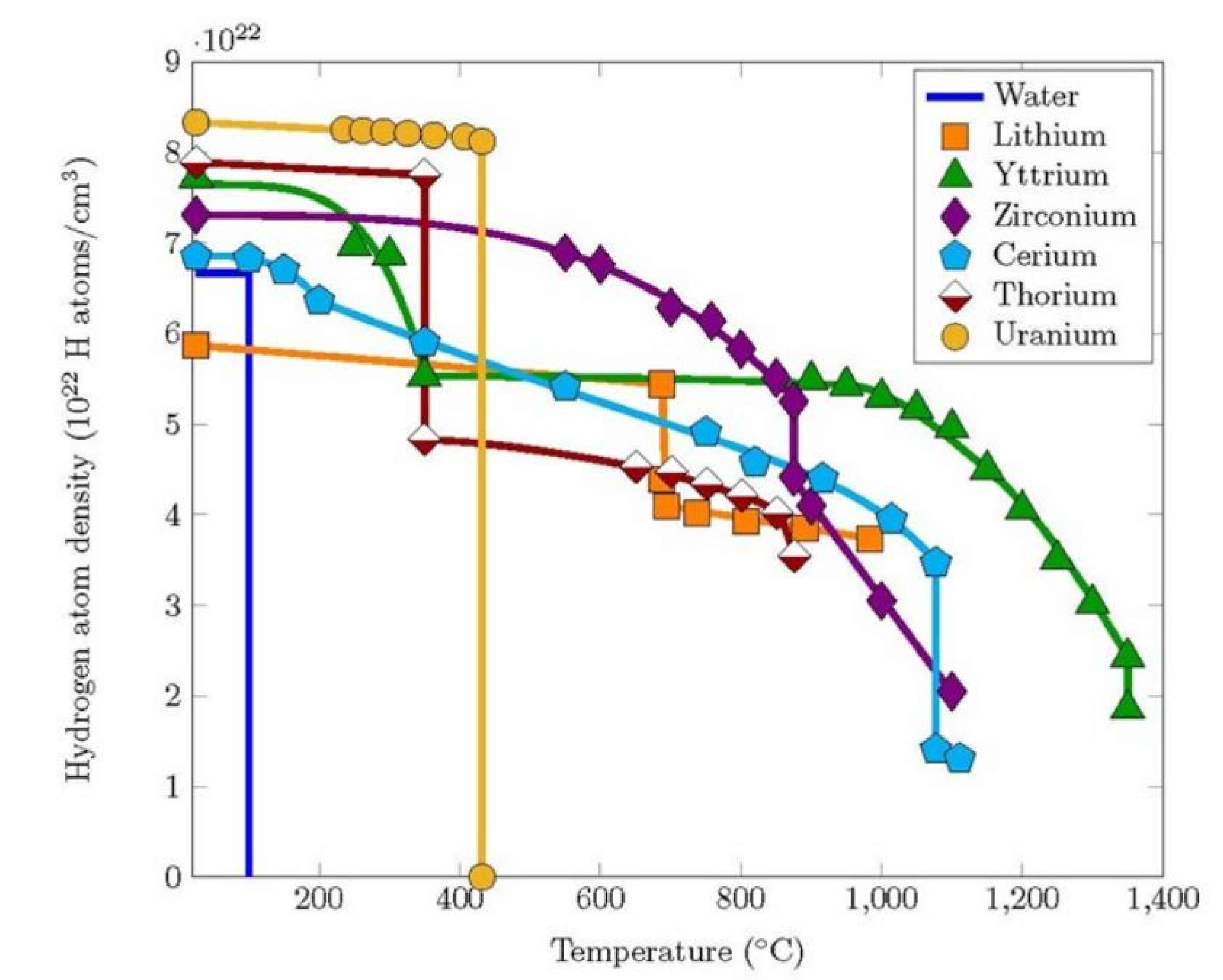
3、 High-Temperature Hydrogen Release

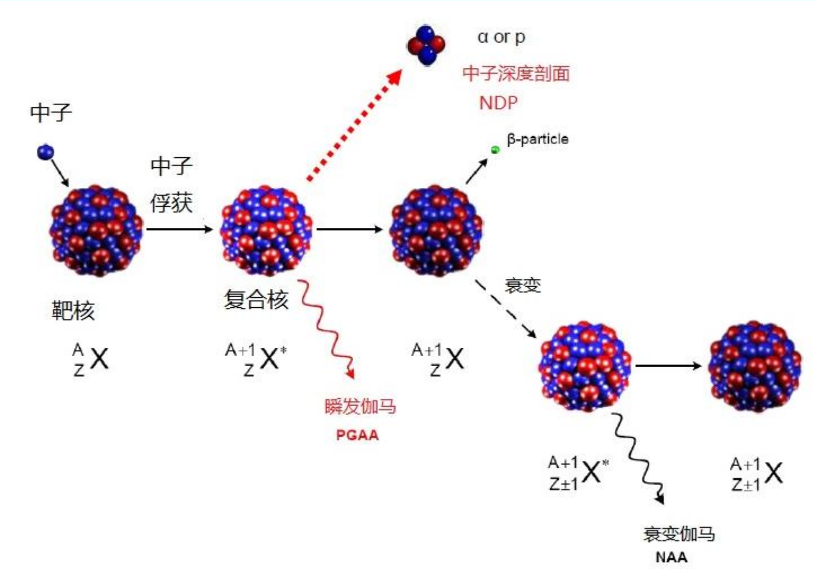
❖ Uranium-Zirconium Hydride: Hydrogen Release Phenomena at Elevated Temperatures



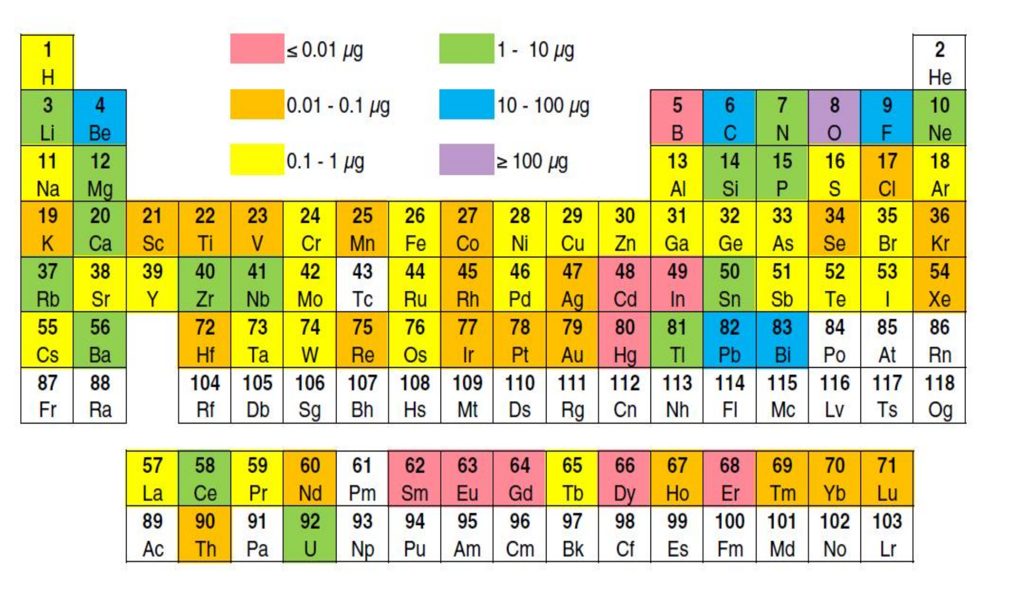


3、 High-Temperature Hydrogen Release

- *To Explore a Novel Method for Hydrogen Release Detection, PGNAA has come into consideration.* PGNAA demonstrates exceptional capabilities as a non-invasive analytical technique, combining high-sensitivity elemental characterization with promising potential for monitoring hydrogen release dynamics in material systems

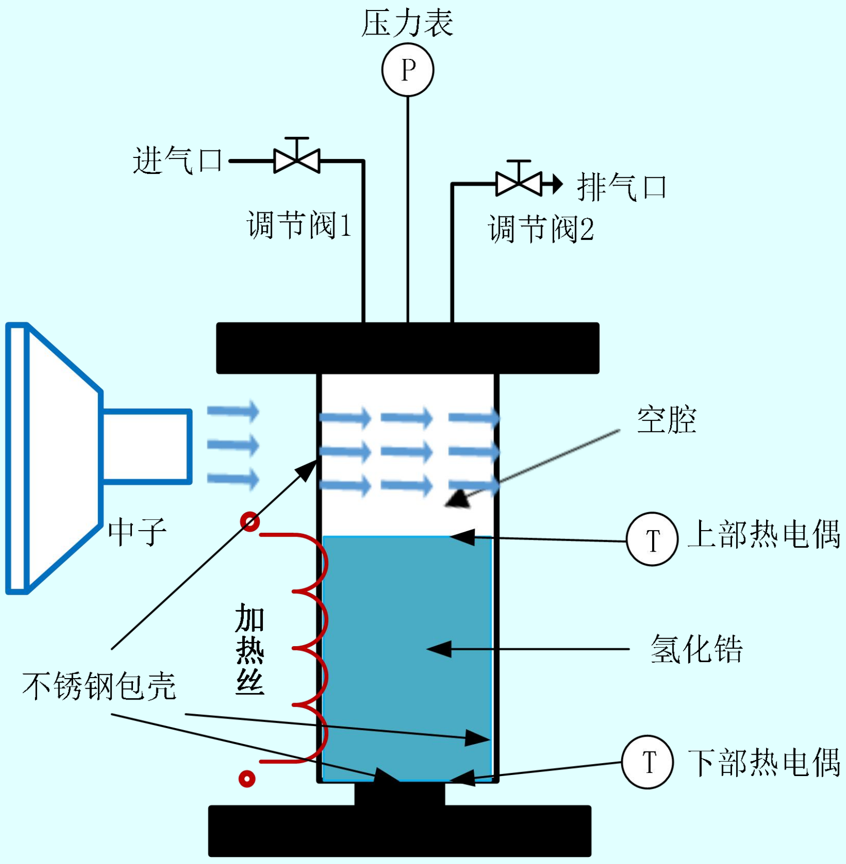


瞬发伽马的产生



瞬发伽马元素探测下限

3、 High-Temperature Hydrogen Release



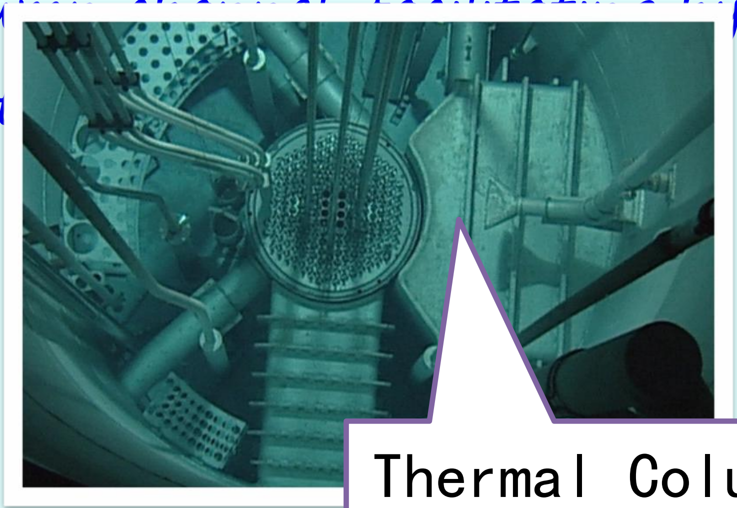
Experiment schematic figure

- Our experiment primarily investigates the hydrogen release mechanisms of zirconium hydride under elevated temperatures. Zirconium hydride metal blocks with an H/Zr ratio of 1.6. A schematic diagram of the experimental setup is provided in Figure 1. The apparatus enables sustained heating of zirconium hydride via heating filaments, with real-time temperature monitoring facilitated by two t

$$^{1}_{1}H + n \rightarrow {}^{2}_{1}H + \gamma \ (2.22\,MeV)$$

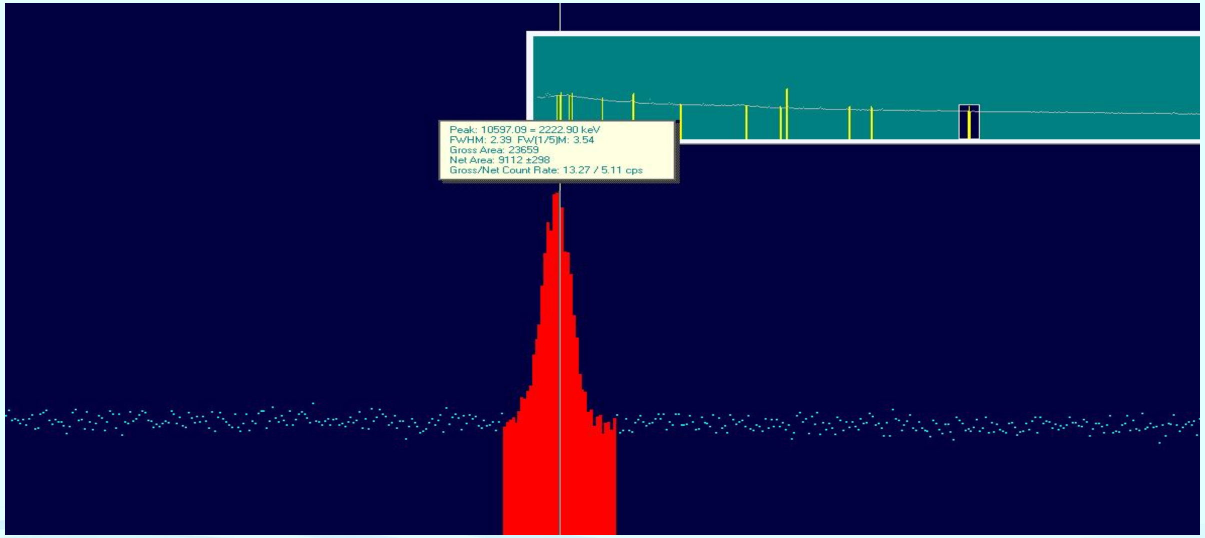
3、 High-Temperature Hydrogen Release

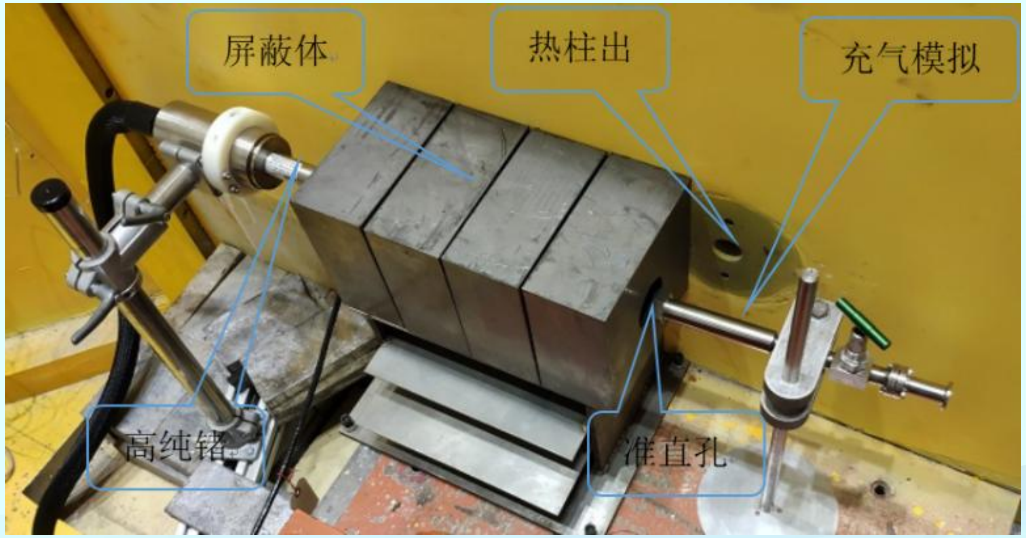
- The thermal column experimental channel of the Xi'an Pulsed Reactor generates a standardized thermal neutron field (Φ35 mm diameter) through a graphite moderator and collimator system, achieving a maximum thermal neutron fluence rate of $1\times10^{5\sim6}$ n·cm^{-2}·s^{-1}. This configuration enables the establishment of a prompt gamma measurement system within the thermal colu … ride ma …



3、 High-Temperature Hydrogen Release

- Performance analysis of the established prompt gamma measurement system was conducted. In this project, a polyethylene sample weighing 38.6 mg (hydrogen content: 5.51 mg) was selected for characterization, with analytical results depicted in the accompanying figure.
- The prompt gamma activation analysis system recorded a full-energy peak of hydrogen at 2223.26 keV, along with a carbon characteristic peak at 1261.71 keV.
- The measured hydrogen full-energy peak count rate reached 0.63 cps (normalized to 0.114 cps/mg). This calibrated value will be utilized in subsequent calculations to quantify hydrogen release from zirconium hydride specimens.

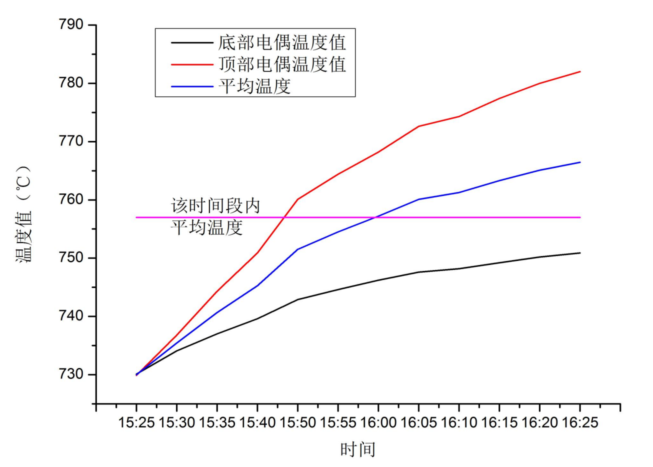


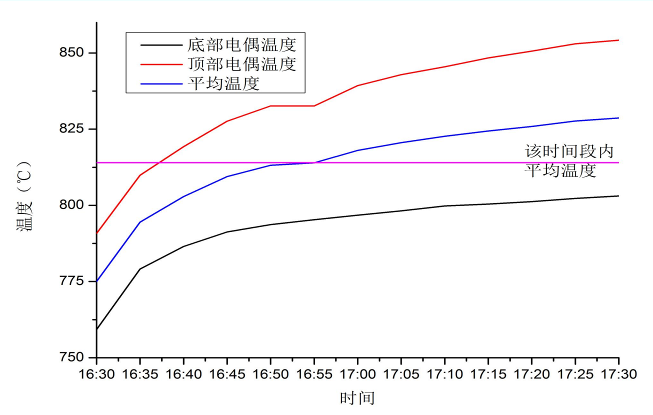


3、 High-Temperature Hydrogen Release

- A dedicated hydrogen release detection was established to investigate the high-temperature hydrogen release characteristics of standard zirconium hydride samples. During full-power reactor operation (2 MW), the prompt gamma activation measurement system accumulated a total measurement duration of 7182 s. The first prompt gamma dataset was captured at 3635 s, corresponding to an average sample temperature of 757 ° C. Continued heating yielded a second measurement upon completion of the thermal cycle, with the zirconium hydride specimen reaching 814 ° C.

Hydrogen release detecting





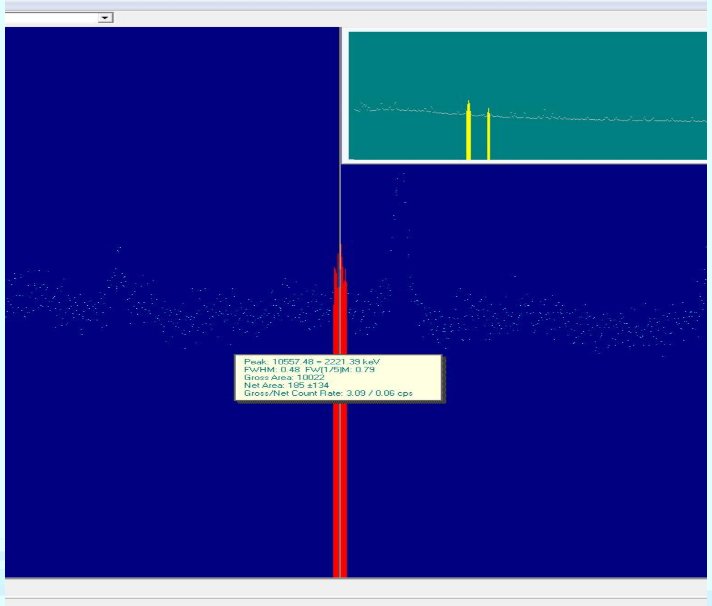
Temp with time

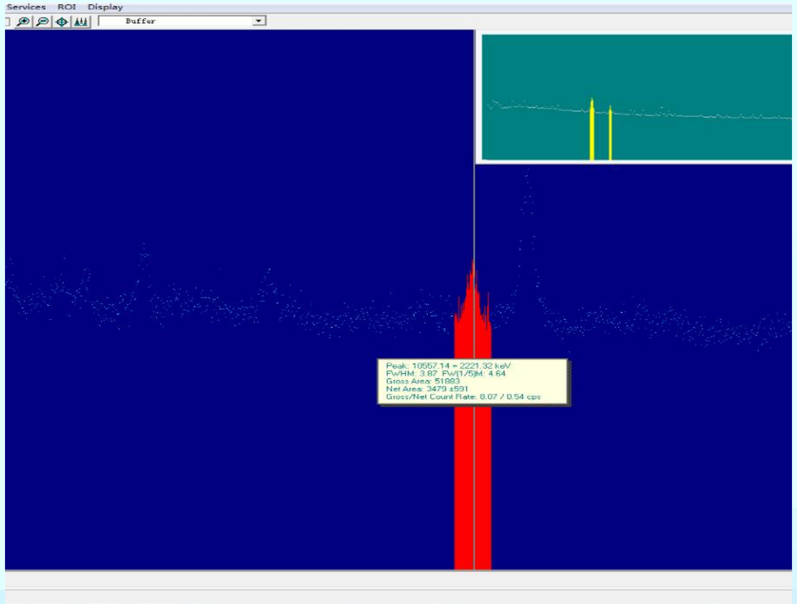
3、 High-Temperature Hydrogen Release

The average hydrogen prompt gamma count rate in the second measurement interval reached 1.04 cps, representing a 16-time increase compared to the initial low-temperature phase. Based on the hydrogen detection efficiency calibration derived from standard reference samples, the hydrogen content within the thermal neutron irradiation field was calculated as 9.02 mg. Assuming a cylindrical neutron flux distribution in the cavity, volumetric correction yields an adjusted hydrogen content of:

$$9.02\times(5.02\times5.0)(3.52\times5.0)=18.408\ \text{mg}.$$

This result aligns with the literature-derived reference value of 17.77 mg obtained from experimental calibration curves.





before After heattig 2 hour

3、 High-Temperature Hydrogen Release

- However, since the PGNAA method relies on high-quality thermal neutron beams, which will cause a certain activation of metal materials, which is not conducive to rapid sample processing and long-term measurement, the next step can be considered to accurately measure the high-temperature hydrogen release content by pressure-composition-temperature (PCT) method, high-resolution mass spectrometry, so as to improve the understanding of the behavior mechanism of zirconium hydride high-temperature hydrogen release.

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4、Hydrogen redistribution

Compared with other hydrogen-containing materials, the metal hydride is characterized by high hydrogen density, which redistributes in the hydride when there are temperature and concentration gradients. The redistribution of hydrogen results in a spatial gradient of hydrogen concentration, which affects the neutron transport in the reactor. There are three driving forces that determine the redistribution of hydrogen in metal hydride, respectively:

(1) diffusion of concentration (Fickian effect) from high concentration zone to low concentration zone;

(2) thermal diffusion (Soret effect) from high temperature zone to low temperature zone;

(3) The stress effect spreads from high compression zone to high tensile zone.(You can ignore it)

The superposition of these three driving forces determines the diffusion flux of hydrogen in the hydride.

$$\rho c_{\mathrm{p}} \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + p_v$$

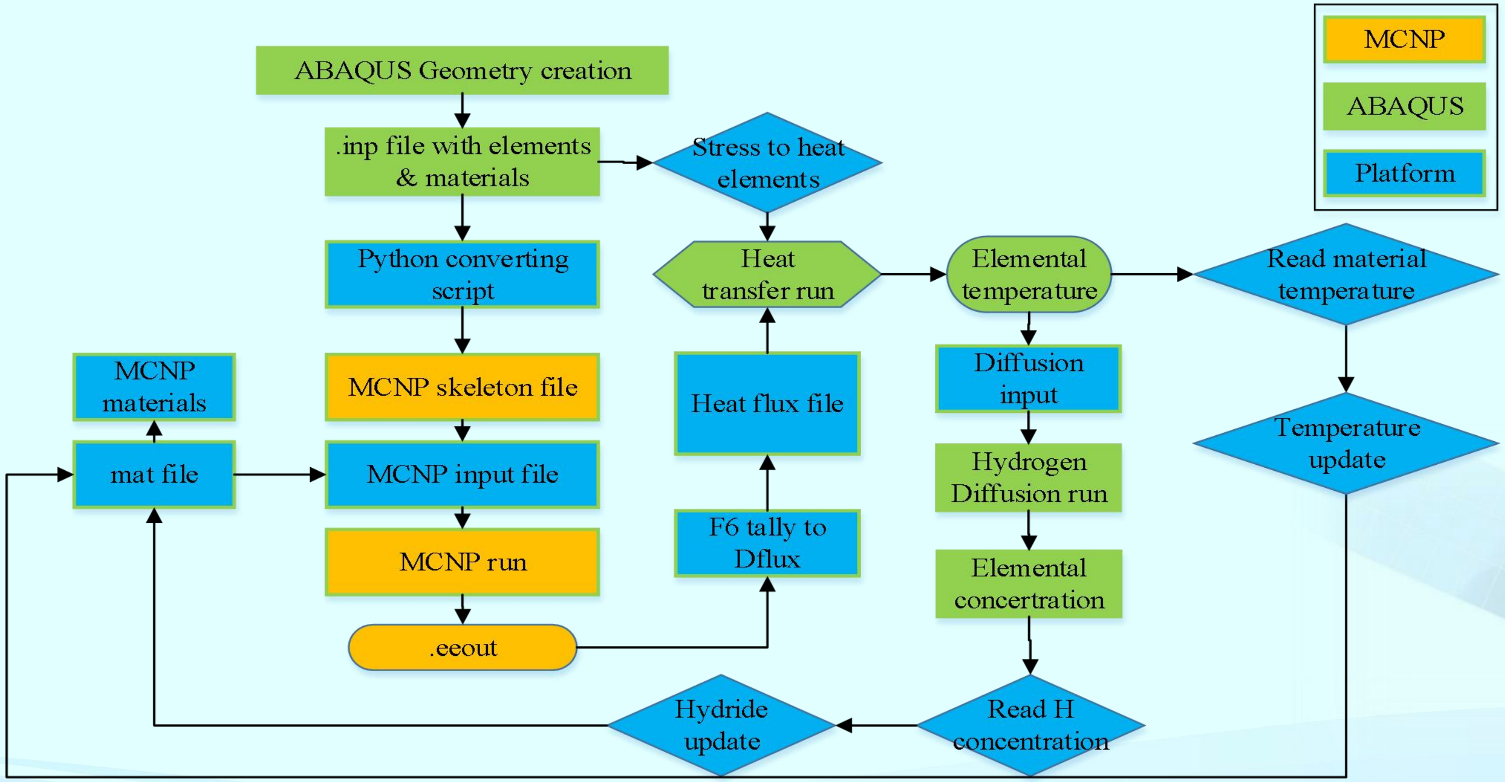
$$J_{\mathrm{H}} = -D[\nabla C + \frac{Q^{*} C}{RT^2} \nabla T - \frac{CV^{*}}{RT} \nabla \sigma]$$

$$J_{\mathrm{H}} = -D \nabla C - D \left(\frac{Q^{*} C}{RT^2} \right) \nabla T$$

$$J_{\mathrm{H}} = -D\left[\nabla C + k_{\mathrm{s}} \nabla \left(\ln\left(T \text{-} \mathrm{T}^{\mathrm{abs}}\right)\right)\right]; \quad k_{\mathrm{s}} = \frac{Q^{*}}{RT^2}$$

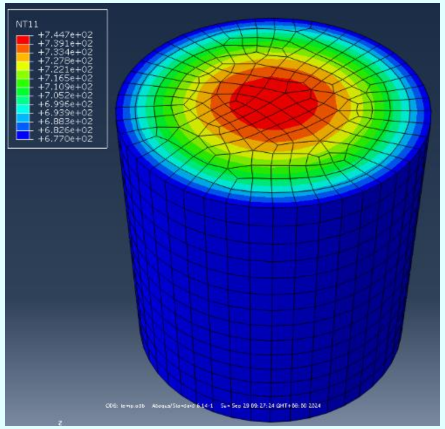
4、Hydrogen redistribution

➢ Three basic physical fields need to be calculated for the high-fidelity hydrogen redistribution model of micro-solid-state reactor: (1) neutronics, (2) heat transfer, (3) mass transfer (or H diffusion), and the combination of MCNP6/DAG-OpenMC based on unstructured grid Monte Carlo program and the finite element software ABAQUS.

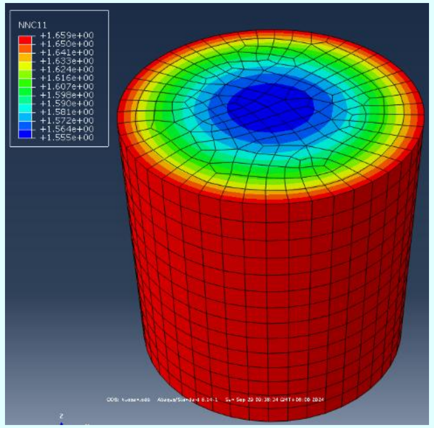


4、Hydrogen redistribution

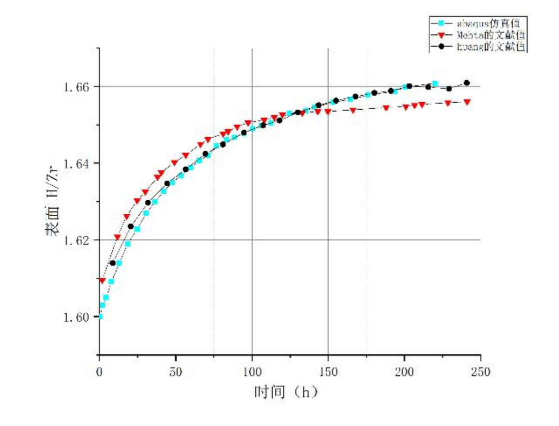
- The modeling data of ABAQUS is consistent with the reference results. When the fuel rod experiences the lowest temperature on the surface, the hydrogen gradually diffuses to the cooler region. So, over time, the hydrogen concentration on the fuel rod's surface increased from 1.60 to 1.66. As a result, the hydrogen concentration seems to reach a steady state value of about 1.66 if the temperature distribution of the fuel rods remains constant. Figure 4 shows the time-dependent variation of hydrogen concentration in UZrHx from the center line of the fuel rod to the surface of the fuel rod.
- Consistent with the reference.



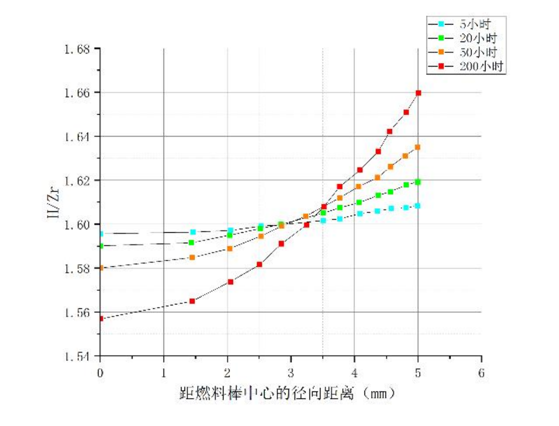
temp



hydrogen



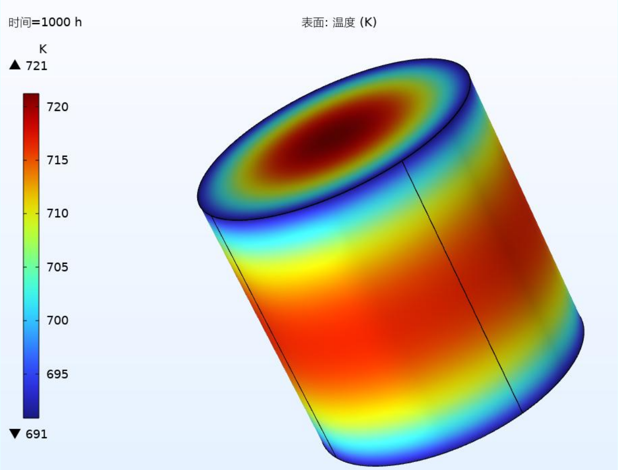
Hydrogen with time



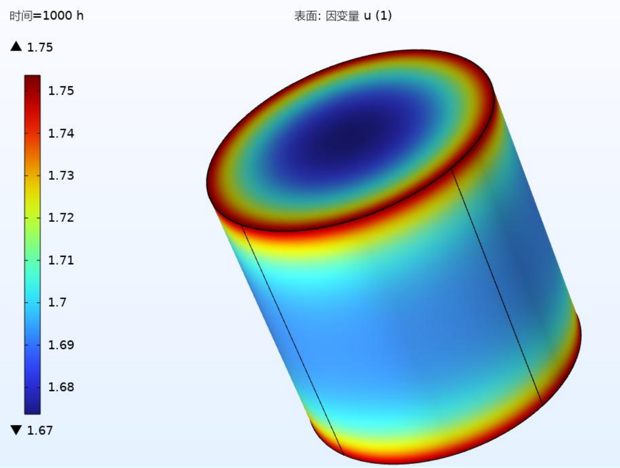
Hydrogen with position

4、 Hydrogen redistribution

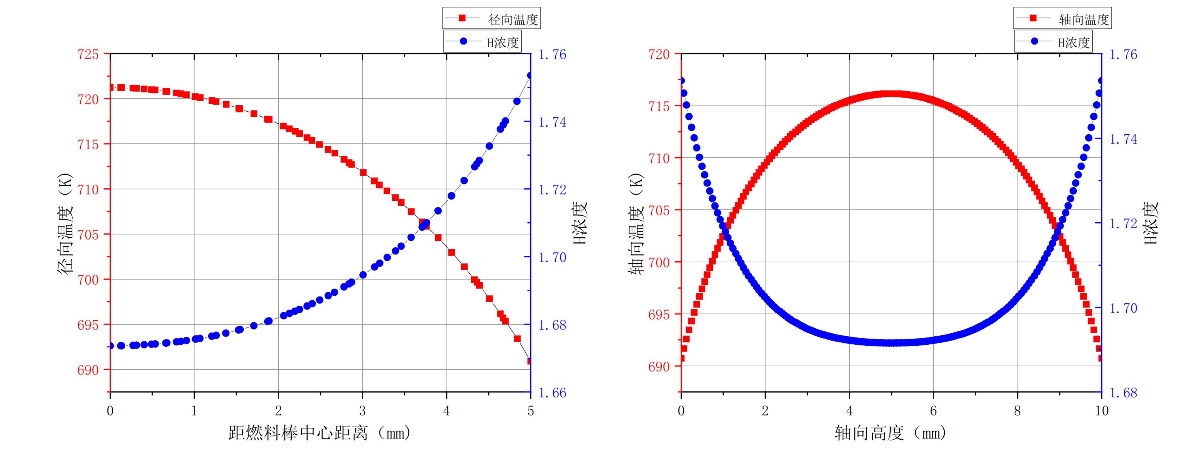
- The upper and lower surface of the fuel core is provided with adiabatic boundary condition in the previous calculation of uranium hydrogen fuel core. Therefore, considering that the upper and lower surfaces are the boundary conditions for heat transfer, the linear heat flux of 300W/ cm is applied to see the steady hydrogen redistribution in this case. When convective boundary conditions are applied to the upper and lower surfaces, the distribution of temperature field is obvious both in radial and axial direction, and the hydrogen atom is still moving from the core region to the low surface area under the drive of temperature gradient.



temp



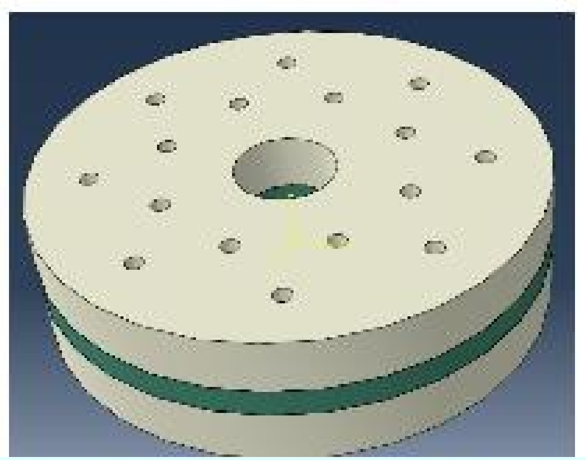
hydrogen



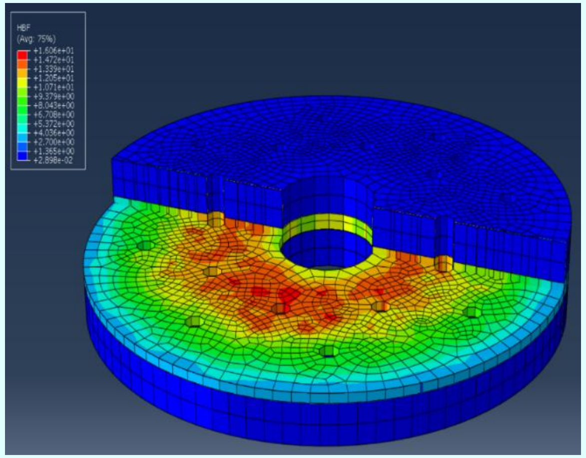
Hydrogen with position

4、 Hydrogen redistribution

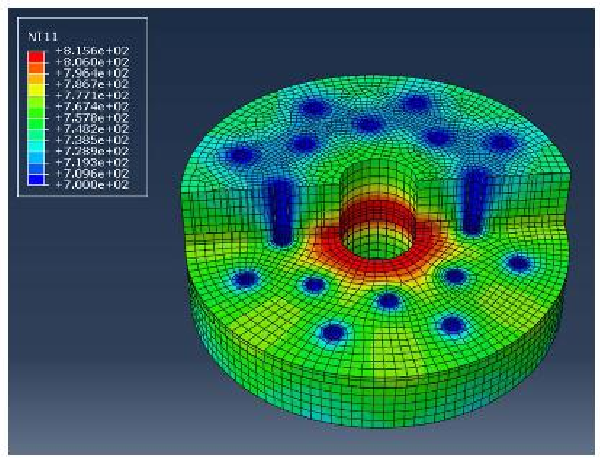
- The characteristics of hydrogen redistribution in sandwich micro solid-state reactor were studied in this paper, similar with the experiment conducted by LANL recently at the National Critical Experimental Research Center, which was used to test the neutron physical properties of hydrogen atoms at high temperatures. Using two layers of YHx disc sandwich high enriched uranium disk, it can be seen that the higher hydride concentration is located near the heat pipe, and the fuel shows zero hydrogen concentration, because there is no hydrogen transfer from moderator to fuel area.



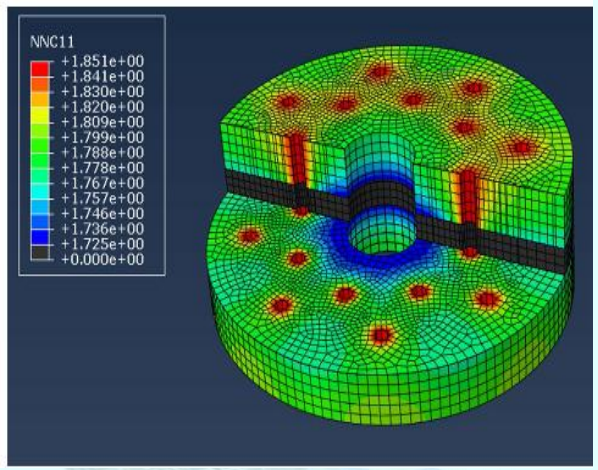
Sanwich reactor



heating



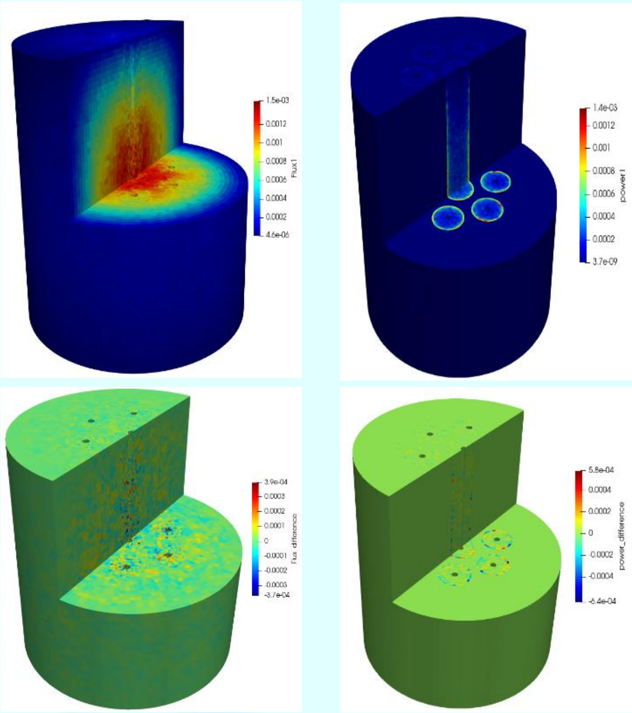
Temp distribution



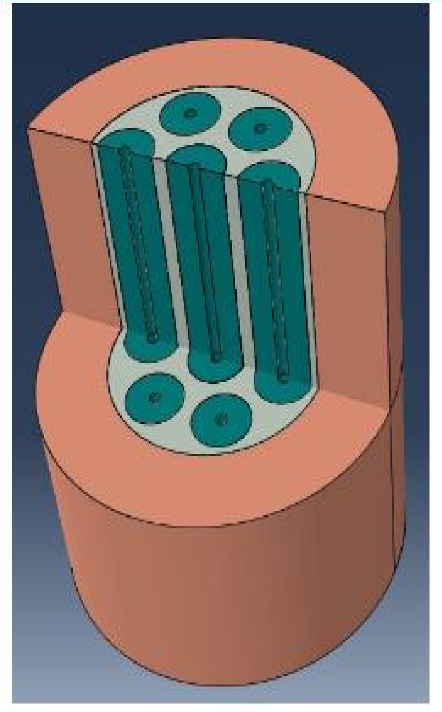
Hydrogen redistribution

4、Hydrogen redistribution

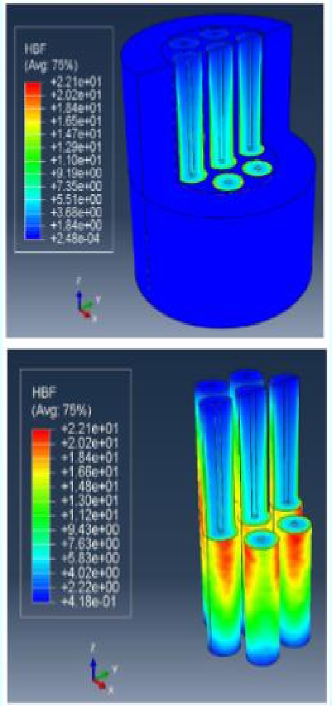
➢ A multi-physical coupling model of nuclear-thermal-hydrogen redistribution for micro solid state reactor with honeycomb coal structure was established. The U-Mo fuel is green, the BeO reflector is orange, and the $YH_{1.8}$ moderator is honeydew color.



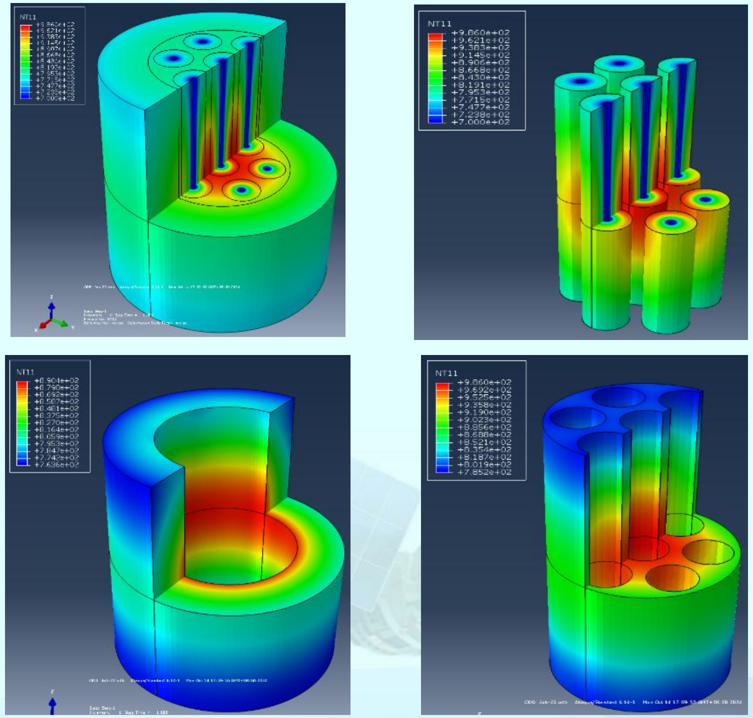
Flux and power distribution



Honeycomb reactor



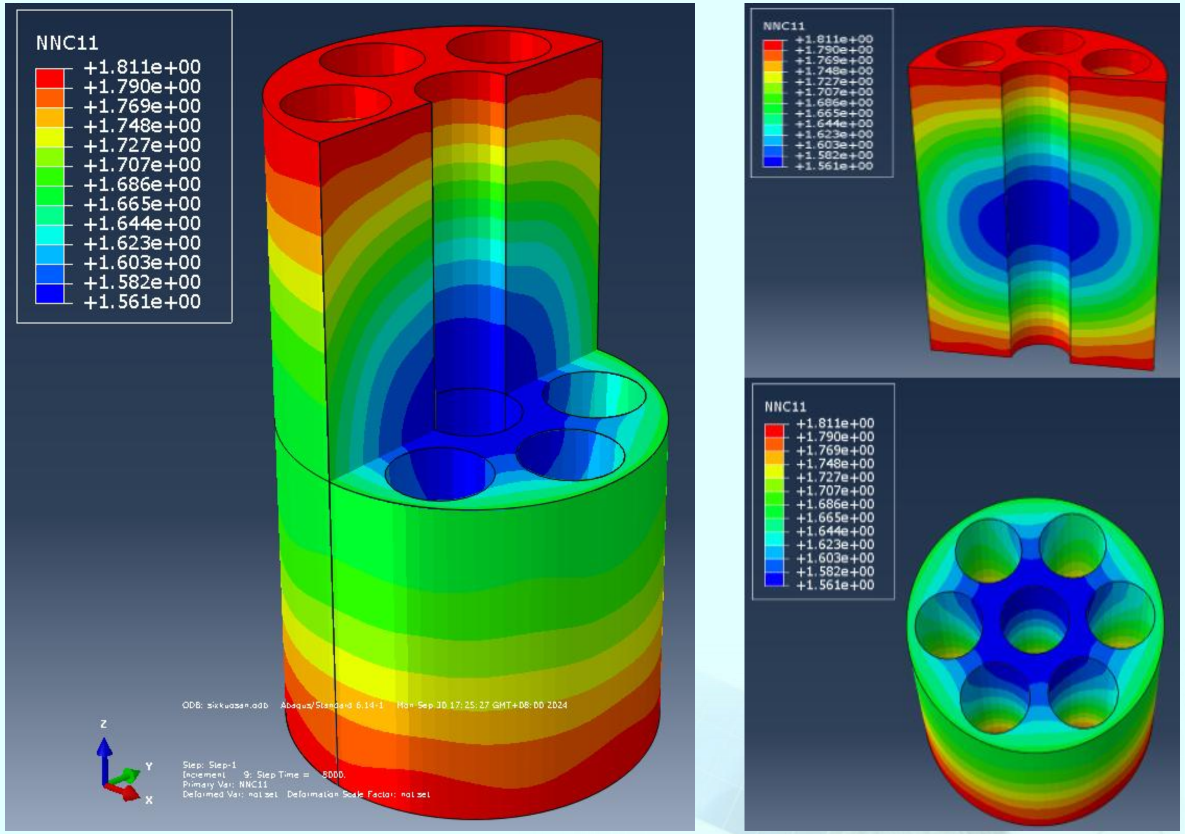
power



Fuel moderator reflector power respectively

4、 Hydrogen redistribution

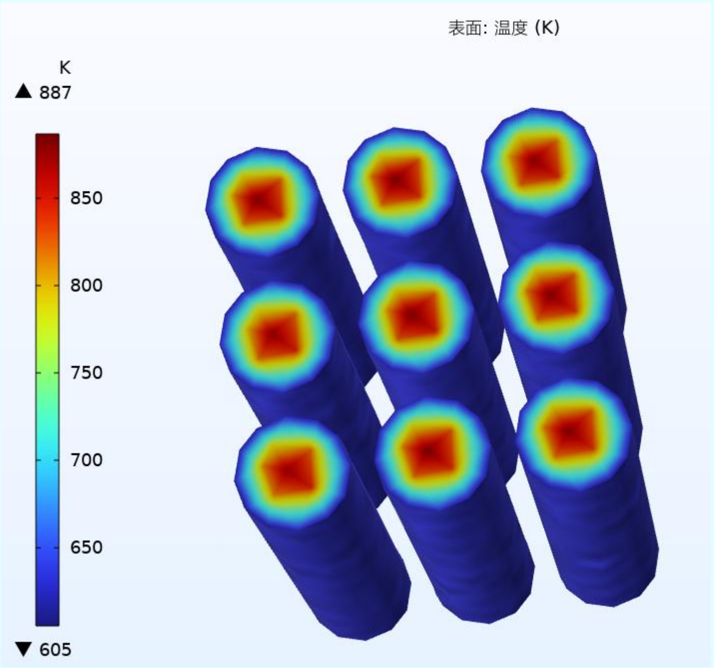
The temperature gradient in the moderator is 193K, and the highest temperature in the moderator region reaches a peak of 983K at the center.
The temperature distribution driven by the Sorret diffusion and the hydrogen concentration distribution drive the Fick diffusion to compete with each other until the net flux of the concentration is zero, the hydrogen redistribution process can be realized in the steady state. The largest H/Y change found was 0.25.Because the Sorret coefficient is positive and hydrogen moves from the higher temperature zone to the cooler region, the lowest concentration of hydrogen is found at the center of the moderator, and the highest concentration of hydrogen is located at the axial ends of the moderator.



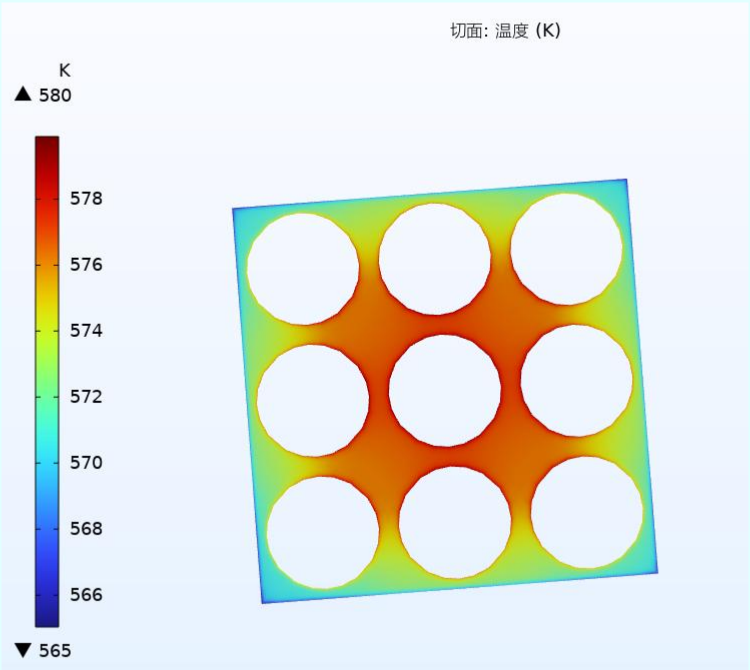
Hydrogen redistribution.

4、Hydrogen redistribution

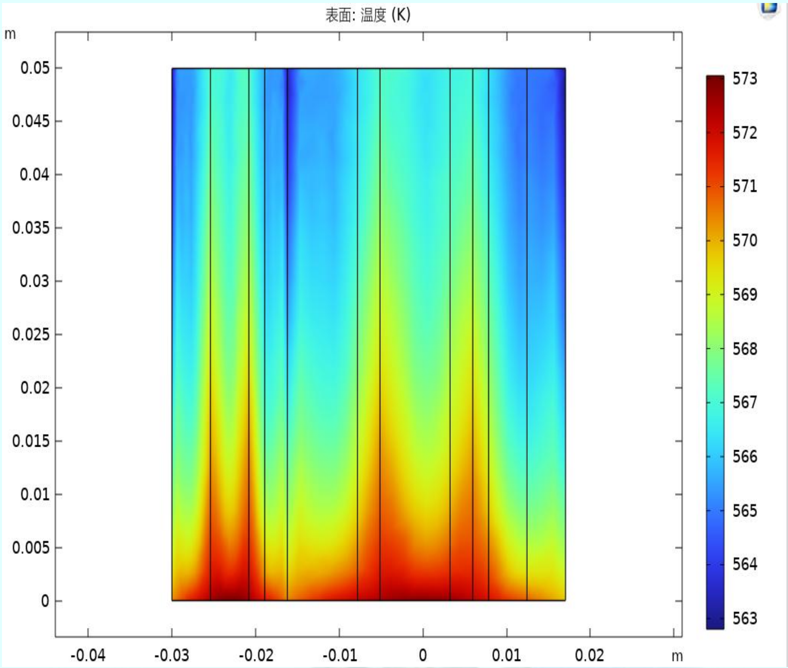
- In order to study the consideration of fluid, the same model of 9x9 uranium hydrogen zirconium assembly was established, and the difference between CFD-hydrogen diffusion and single channel-hydrogen redistribution was compared. The following is the solid heat transfer and CFD results.



Fuel temp



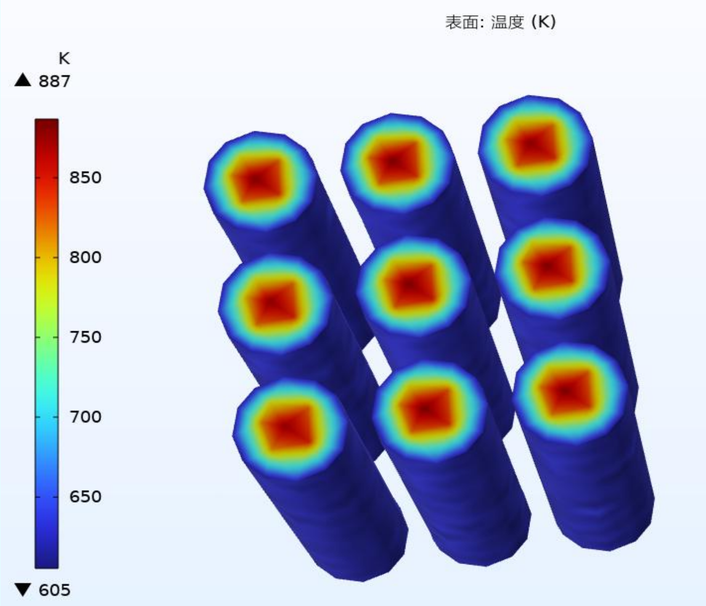
Coolant temp



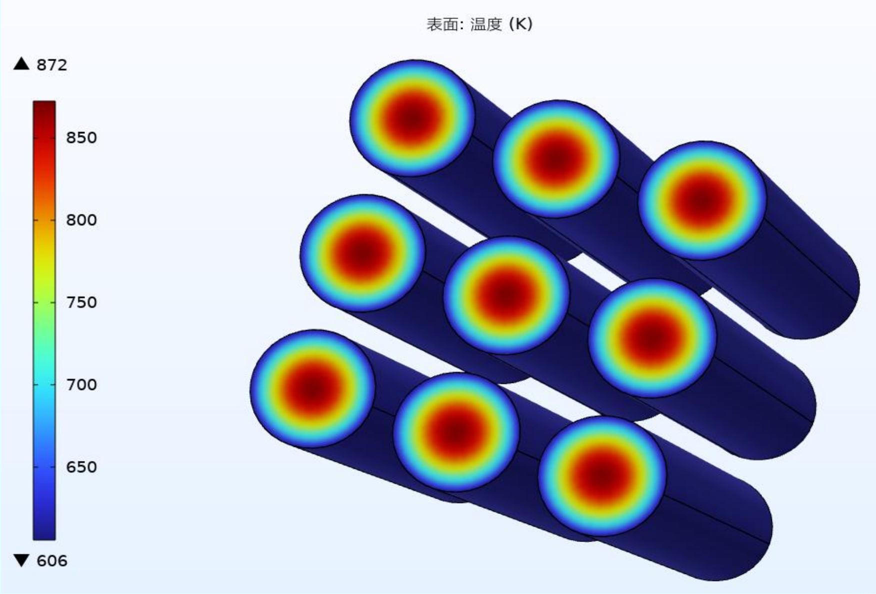
Coolant temp

4、Hydrogen redistribution

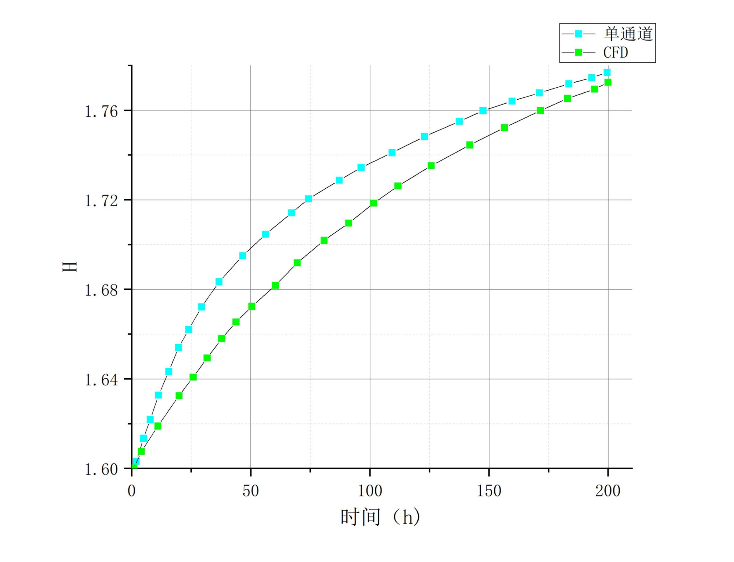
- Compared with the temperature distribution of fuel rods calculated by CFD and single channel method, it can be seen that the difference between the two is small and the model is basically accurate. At the same time, the calculation of 9x9 fuel assembly model using single channel method takes only 3 seconds, which greatly improves the calculation efficiency and simplifies the calculation flow.



CFD



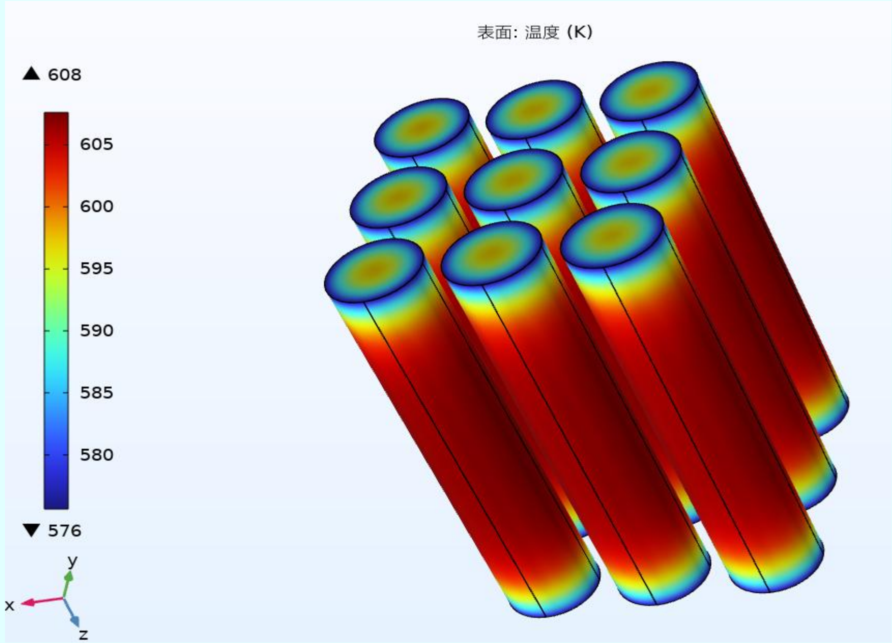
single channel method



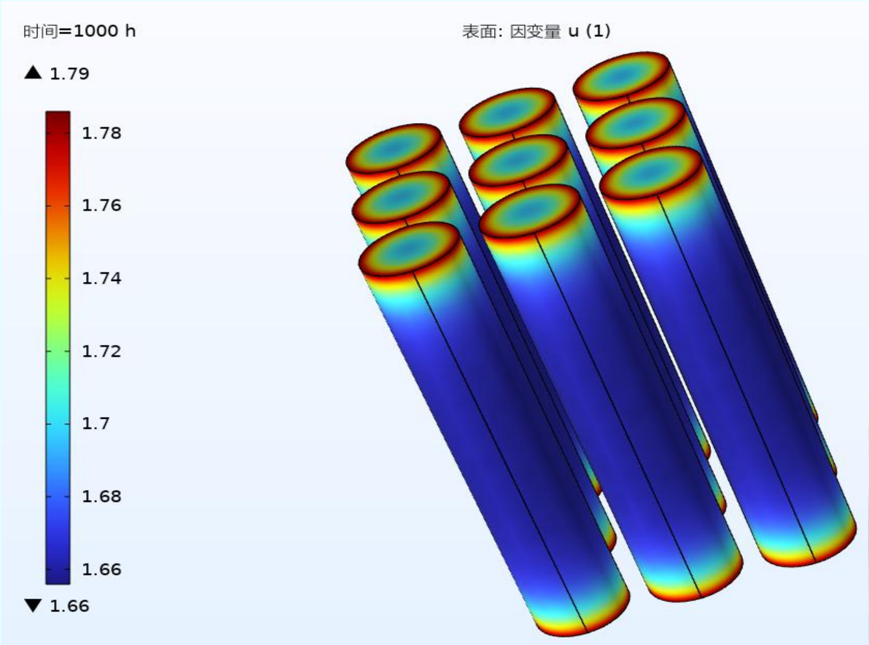
Comparison with time

4、 Hydrogen redistribution

- For the nine-bar case, the upper and lower surfaces are considered as the boundary conditions for heat transfer. A single channel method is adopted to calculate the linear heat flux of 100W/ cm, and similar results are obtained.

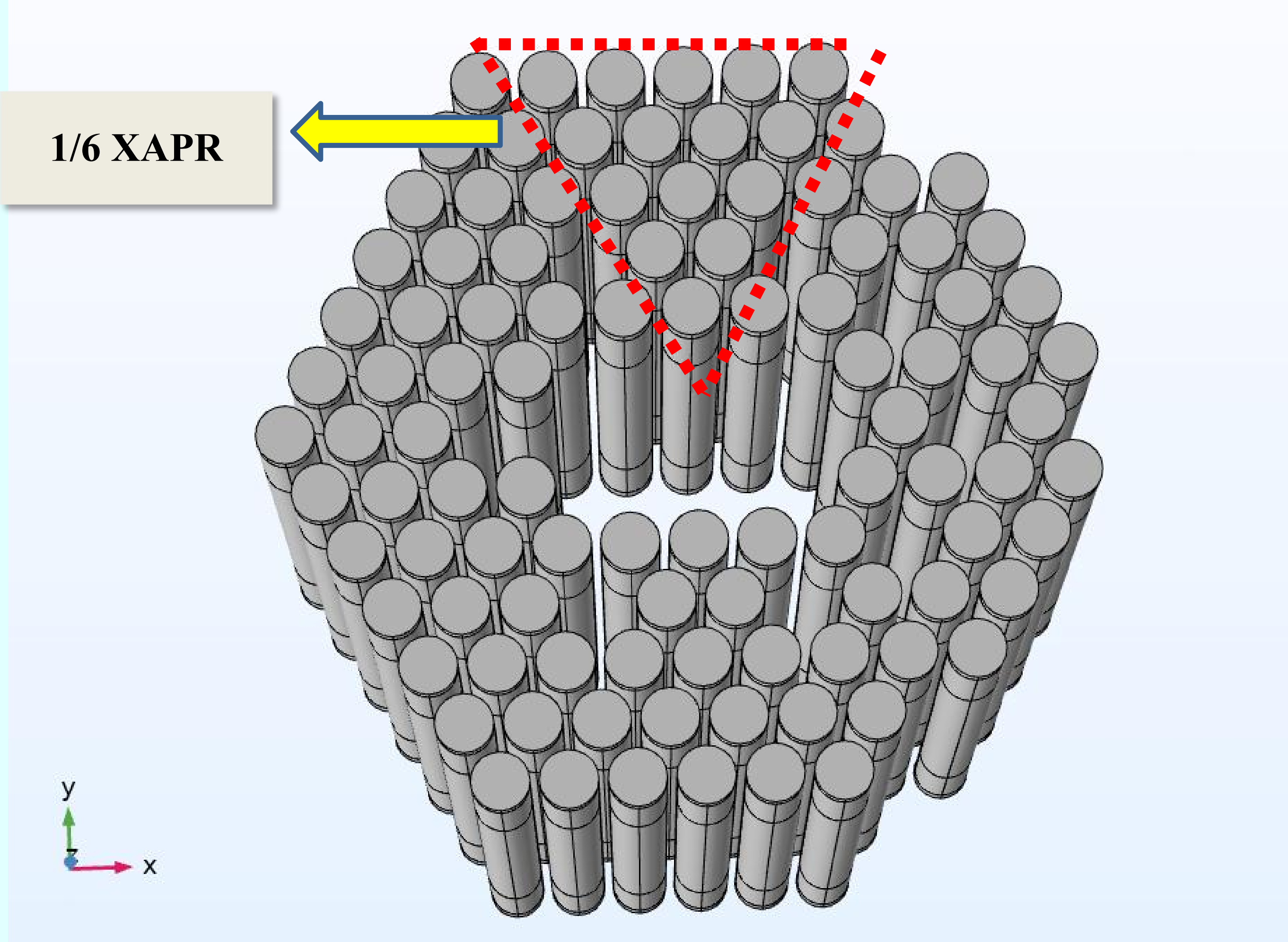


temp

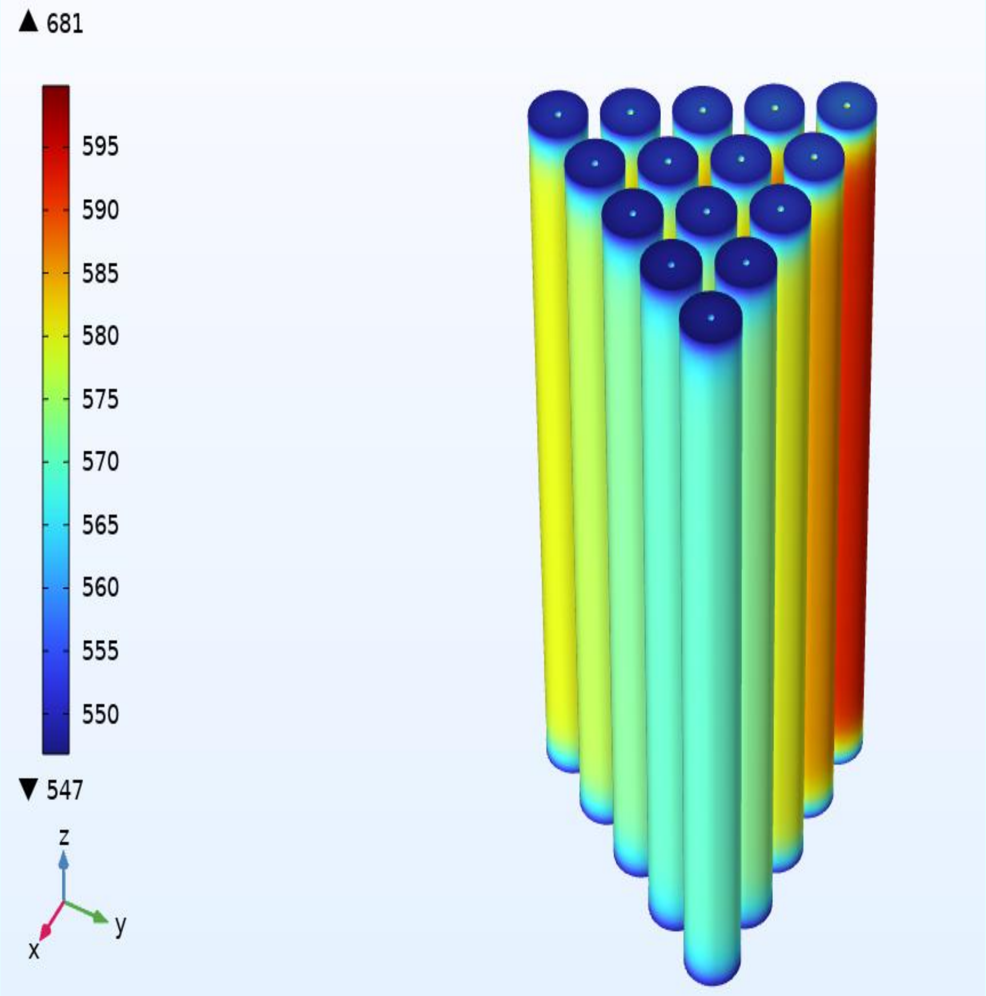


hydrogen

4、 Hydrogen redistribution

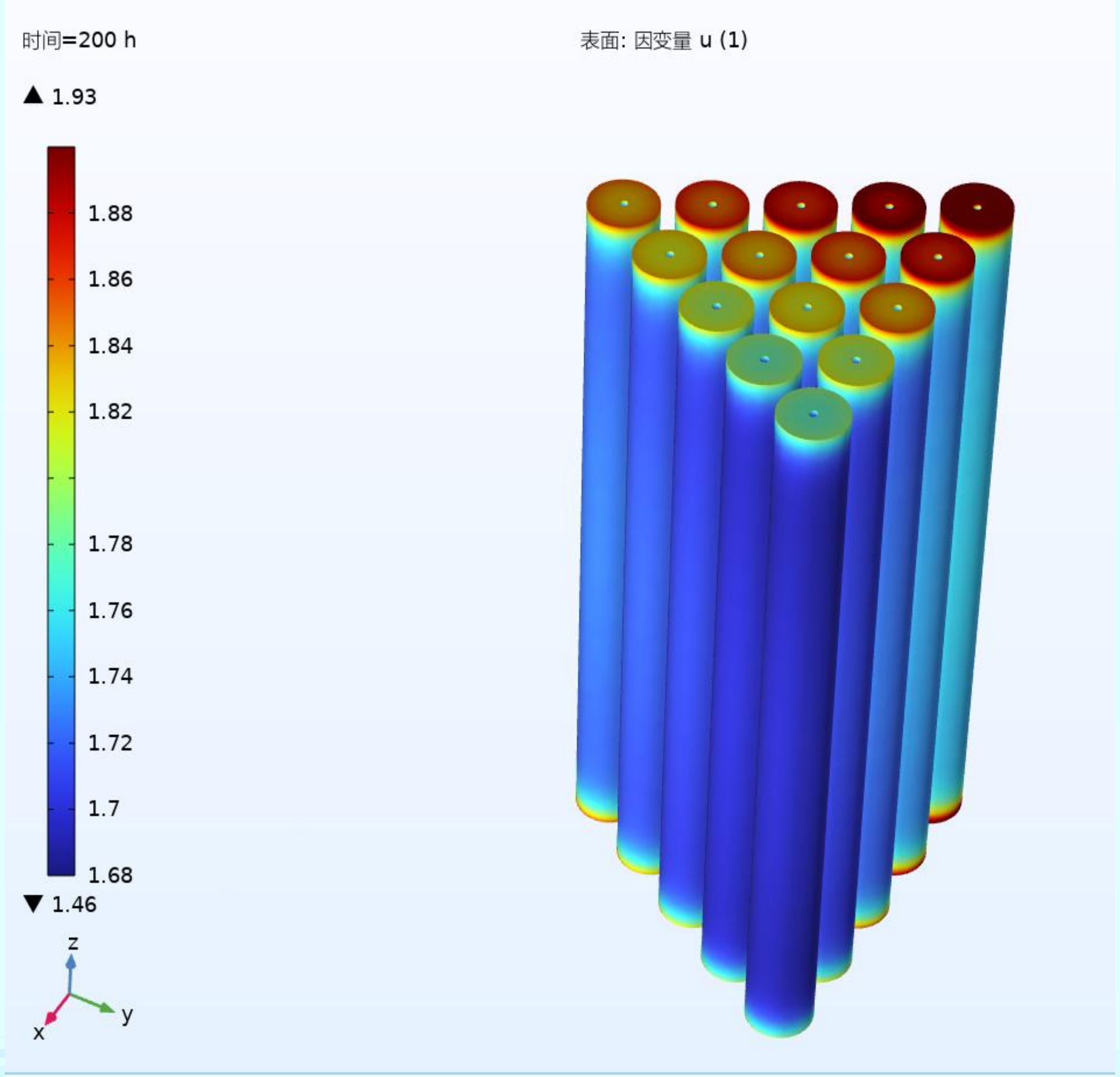


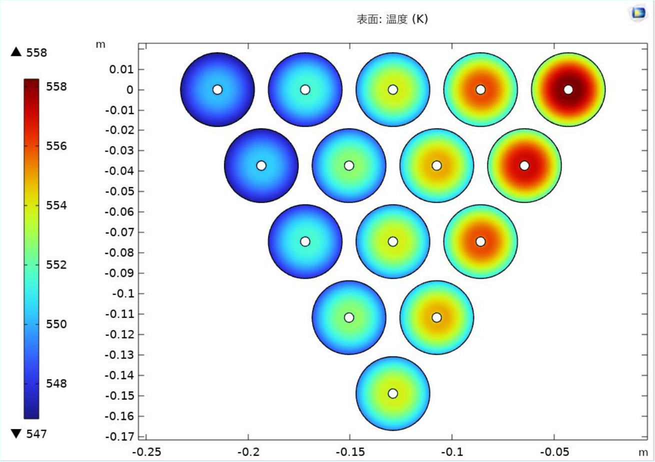
Xi’an Pulsed reactor



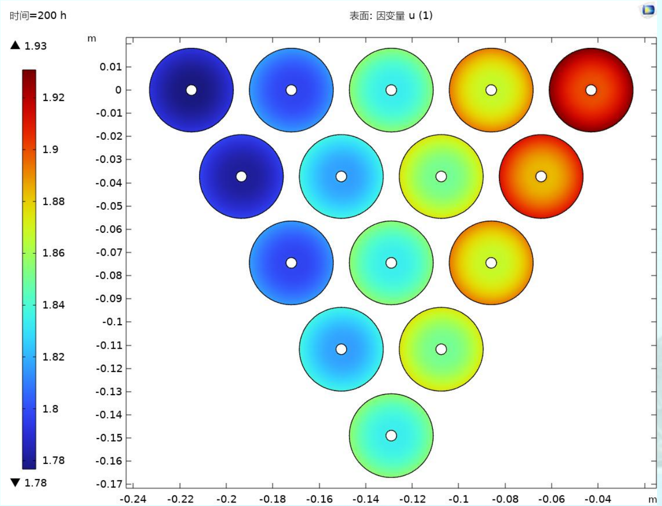
Temp distribution

4、 Hydrogen redistribution





Temp distribution



Hydrogen distribution

CONTENTS

5、Summary

❖ **Summary**

- The nuclear safety problems involved in the application of metal hydride in micro-reactor are studied and combed systematically. The thermal mechanism, hydrogen release and hydrogen redistribution characteristics are put forward.
- The mechanism of neutron thermalization of metal hydride moderator in micro-reactor was studied, and the neutron thermal effect of metal hydride was studied from the angle of first principle.
- High-accuracy measurements of high-temperature hydrogen release from metal hydrides were conducted using a prompt gamma activation analysis (PGNAA) system, providing reliable experimental data on their hydrogen release characteristics under elevated thermal conditions
- The study on the multi-physical coupling of hydrogen redistribution characteristics of metal hydride is established, which lays an important theoretical foundation for the systematic study of its nuclear safety behavior.

Thank you!