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Transforming Microreactor Economics Through Hydride Moderator Enabled Neutron Economy

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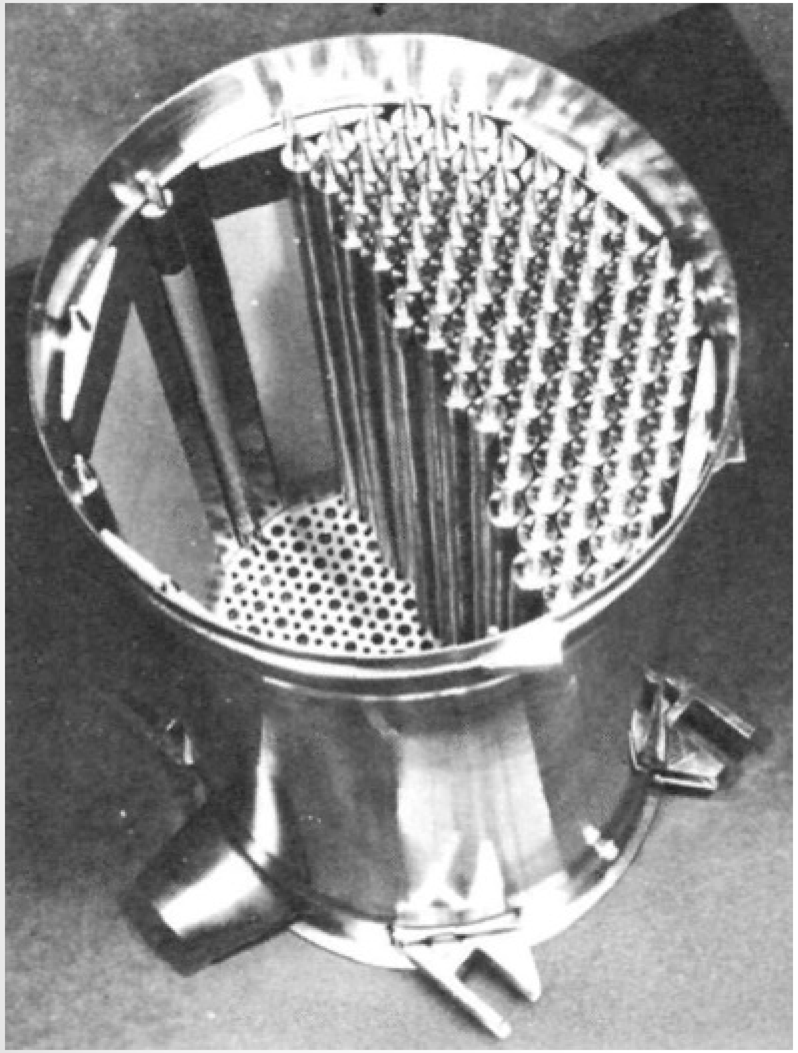
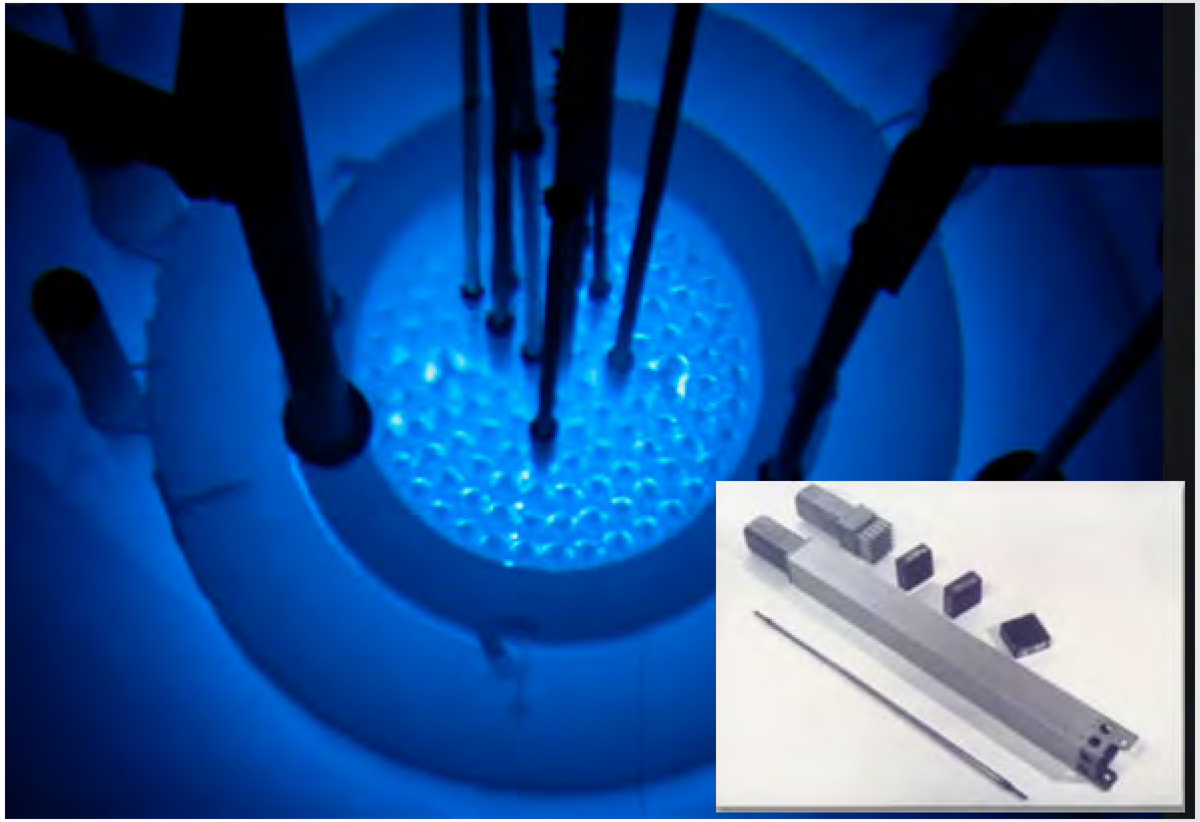
Metal hydrides have also been explored as moderators

Aircraft Reactor Experiment-1954

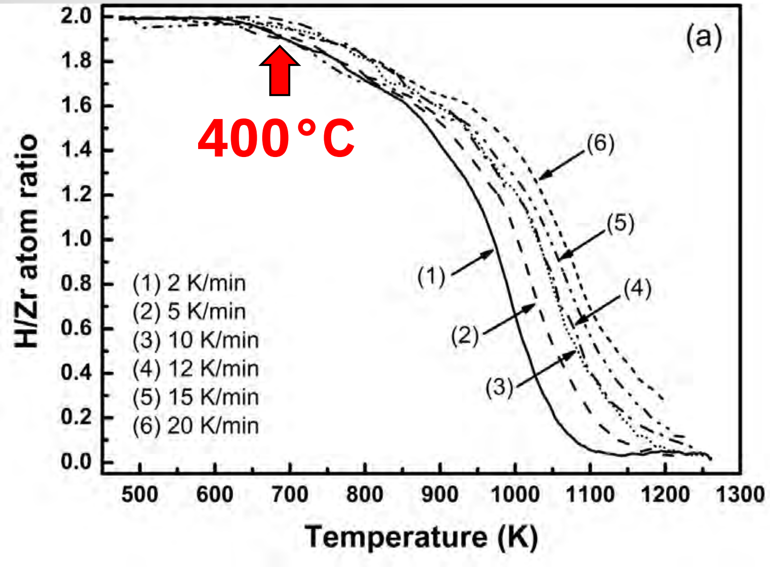


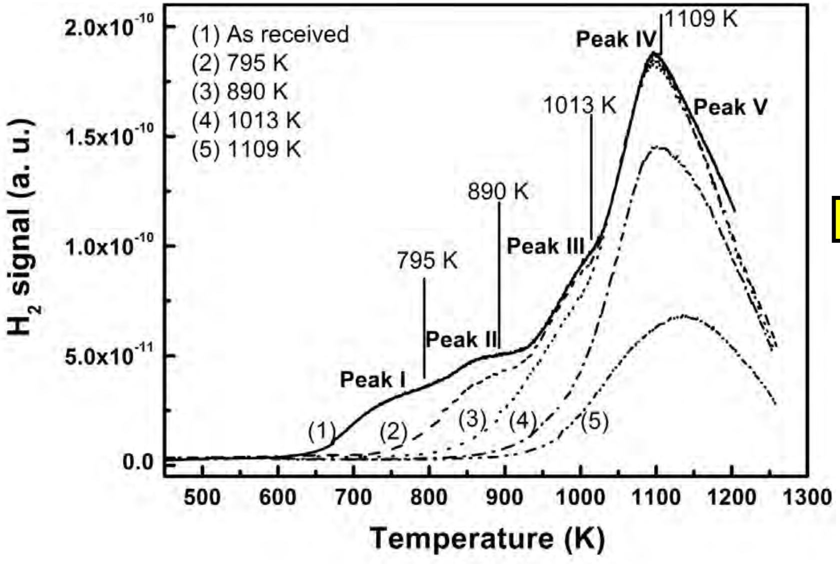
Mixed Zirconium Hydride-Uranium TRIGA Fuel

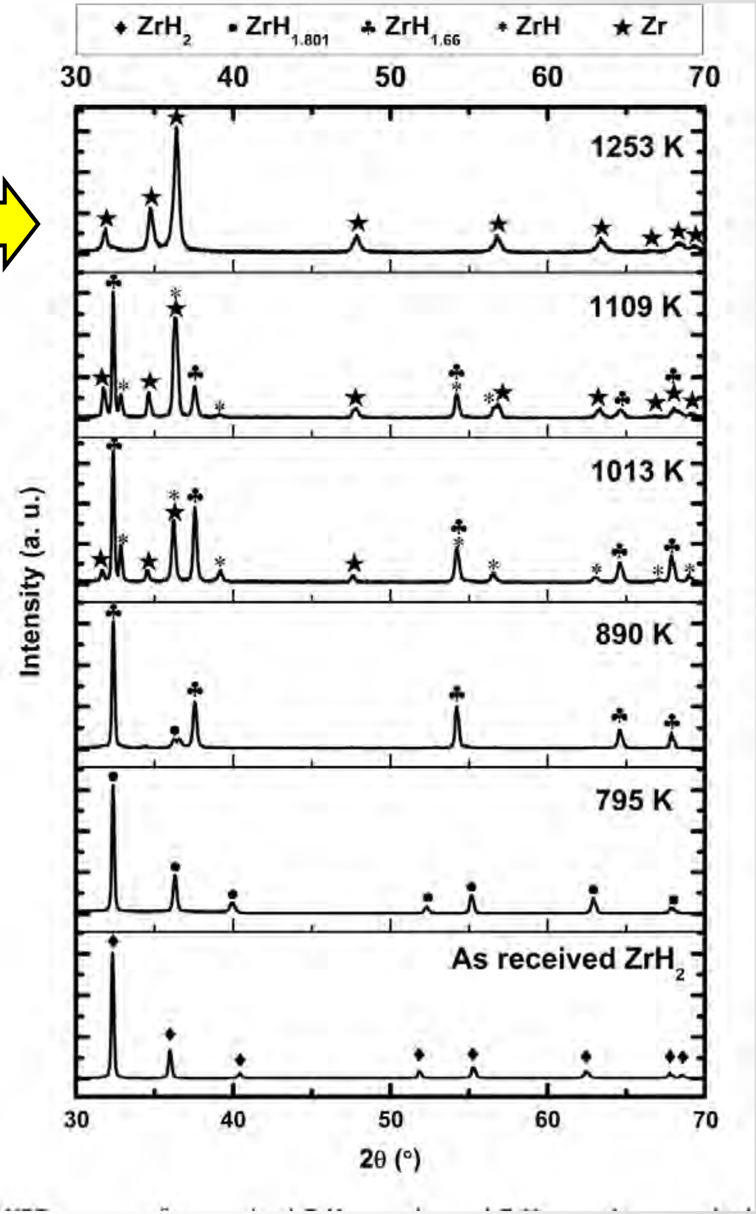


Metal hydrides have hydrogen content approaching water, thus are very good moderators, but tend to decompose at elevated temperature and under irradiation

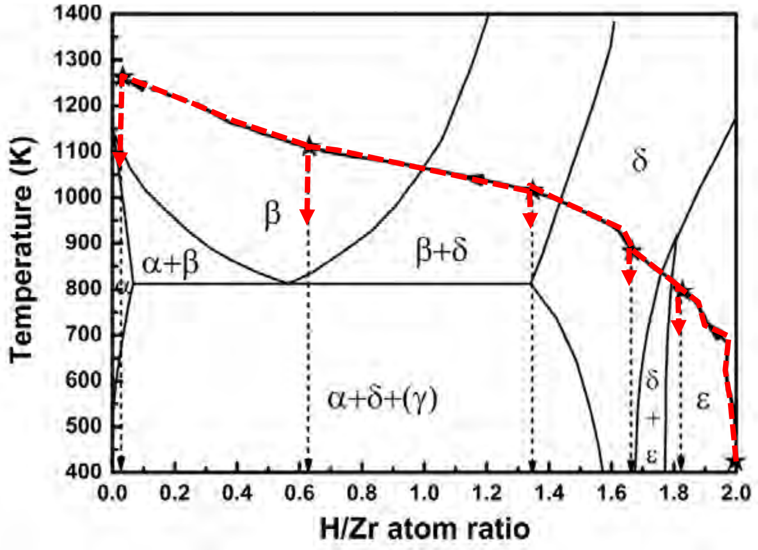
Background: thermodynamic limitations of ZrH_x







$$\varepsilon \rightarrow \delta+\varepsilon \rightarrow \delta \rightarrow \beta+\delta \rightarrow \beta$$



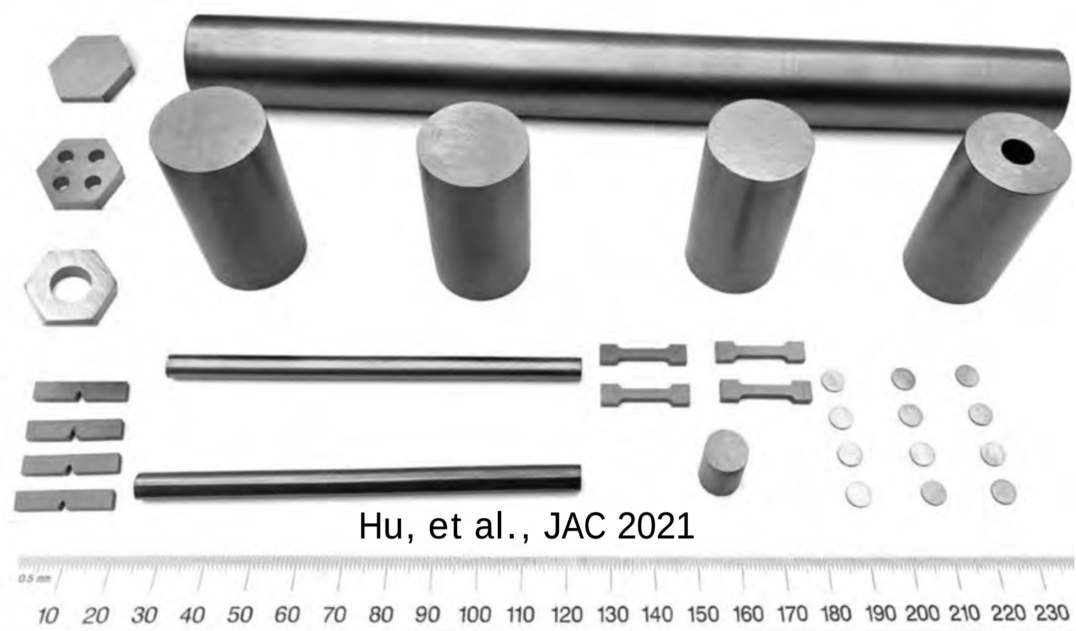
Hydride stability is intrinsically limited by thermodynamics, but what if we can suppress the desorption of hydrogen?

Ma et al. JAC 2015

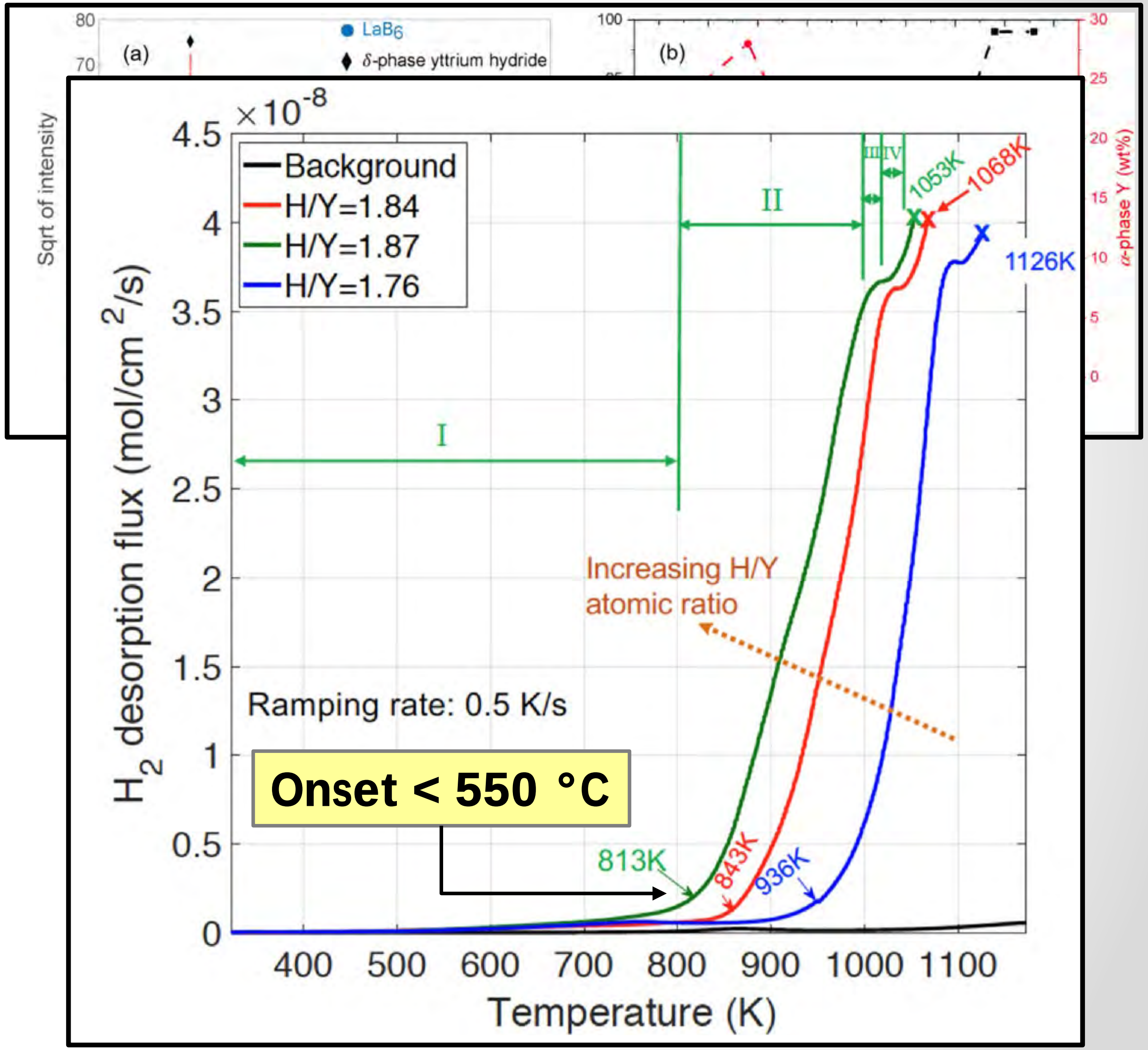
What about using different candidate hydrides?

Hu, et al., JNM 2020

Hydride	Attainable hydrogen density 10^{22} atoms H/cm^3	Attainable hydrogen density g H/cm^3	Hydride density (g/cm^3)	Slowing down power	Moderating 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
H_2O	6.6	0.110	0.98	1.35	70
$ThZr_2H_7$	7.7	0.129	7.75	1.55	14
$ThTi_2H_6$	8.8	0.147	8.15	1.8	6



Hu, et al., JAC 2021



Trofimov, et al., JNM 2020

Ceramic composites as engineered moderator/reflector materials

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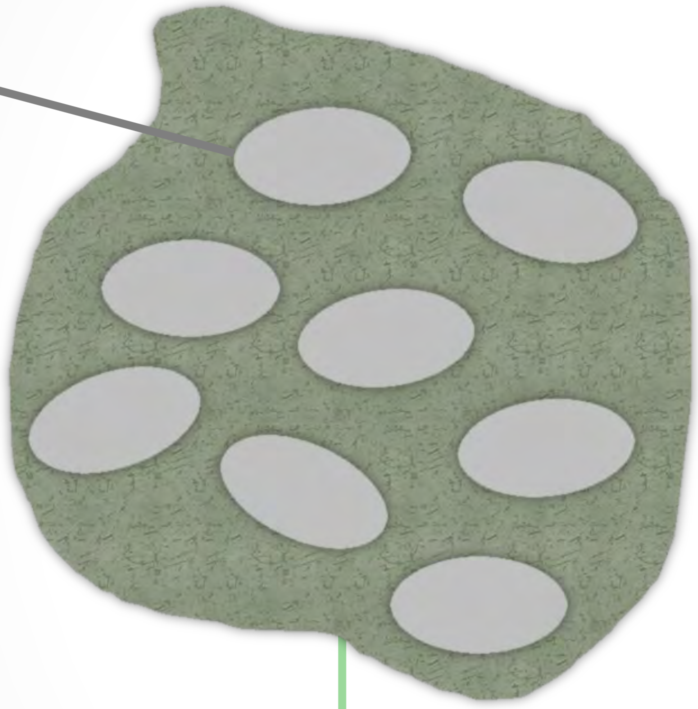
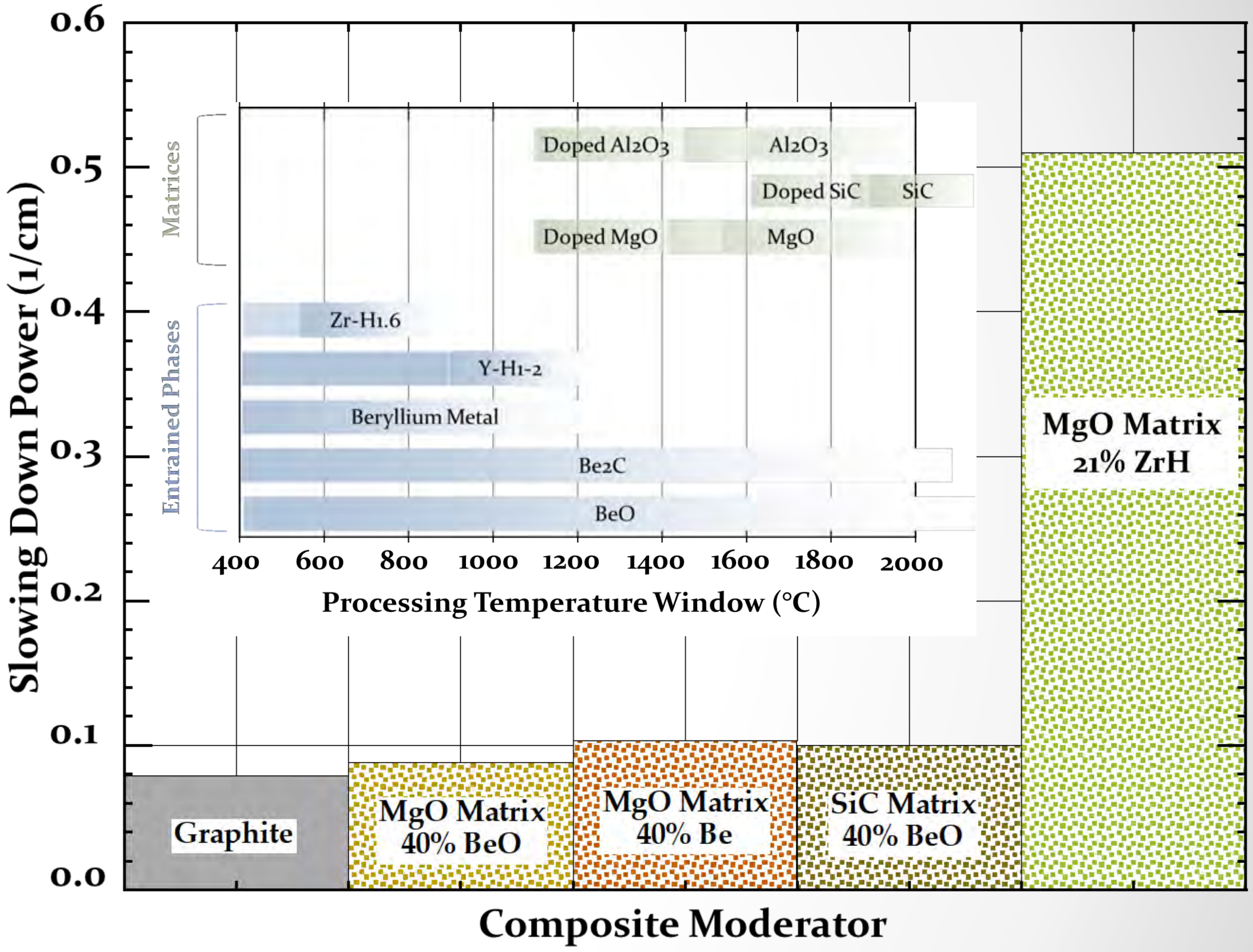
Entrained Phase
- High Moderation
- Low Neutron Absorption
- Fair Radiation Stability
- Low Transmutation



Matrix Phase
- Fair Moderation
- Low Absorption
- Good Radiation Stability
- Good Thermal Conductivity
- Good Compressive Strength
- Low Permeability



Manufacturing: ideally no chemical reactivity between the two phases with processing temperatures that do not decompose either phase and offer a pathway to economy of scale.

Project goals and objectives

Goals

- Demonstrate significantly reduced fuel costs through novel microreactor designs enabled by the technical advancement of engineered hydride ceramic composite moderators.

Objectives

1. Fabricate stabilized entrained hydride moderators for continuous operation at 800 °C through neutronics informed optimization
2. Enhance the performance of an annular, spherically-shaped, and reflected core through these moderators and integrated design optimization
3. Produce entrained hydride composites up to 10 cm in diameter via DCS and map the spatial distribution of microstructure and properties,
4. Measure H desorption from the entrained hydride composites with a migration model developed for hydrogen transport in MgO
5. Quantify the trade-off cost with savings realized through reduced uranium loading and other factors pertinent to microreactors.

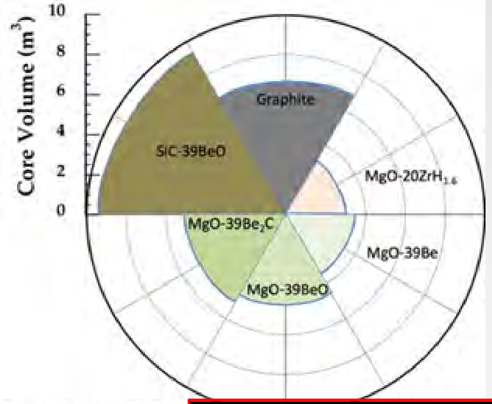
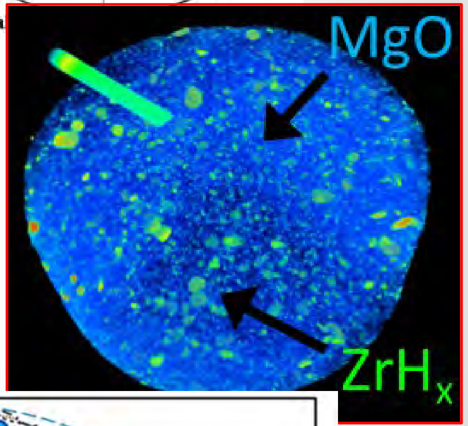
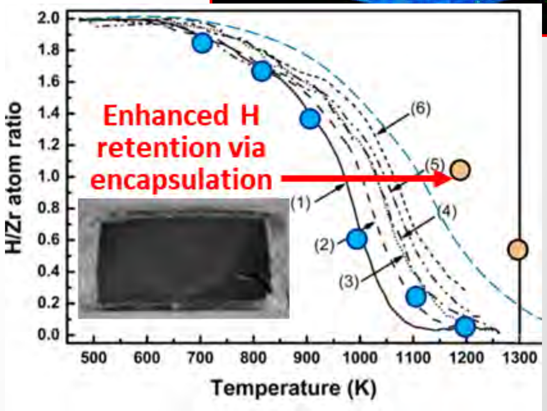
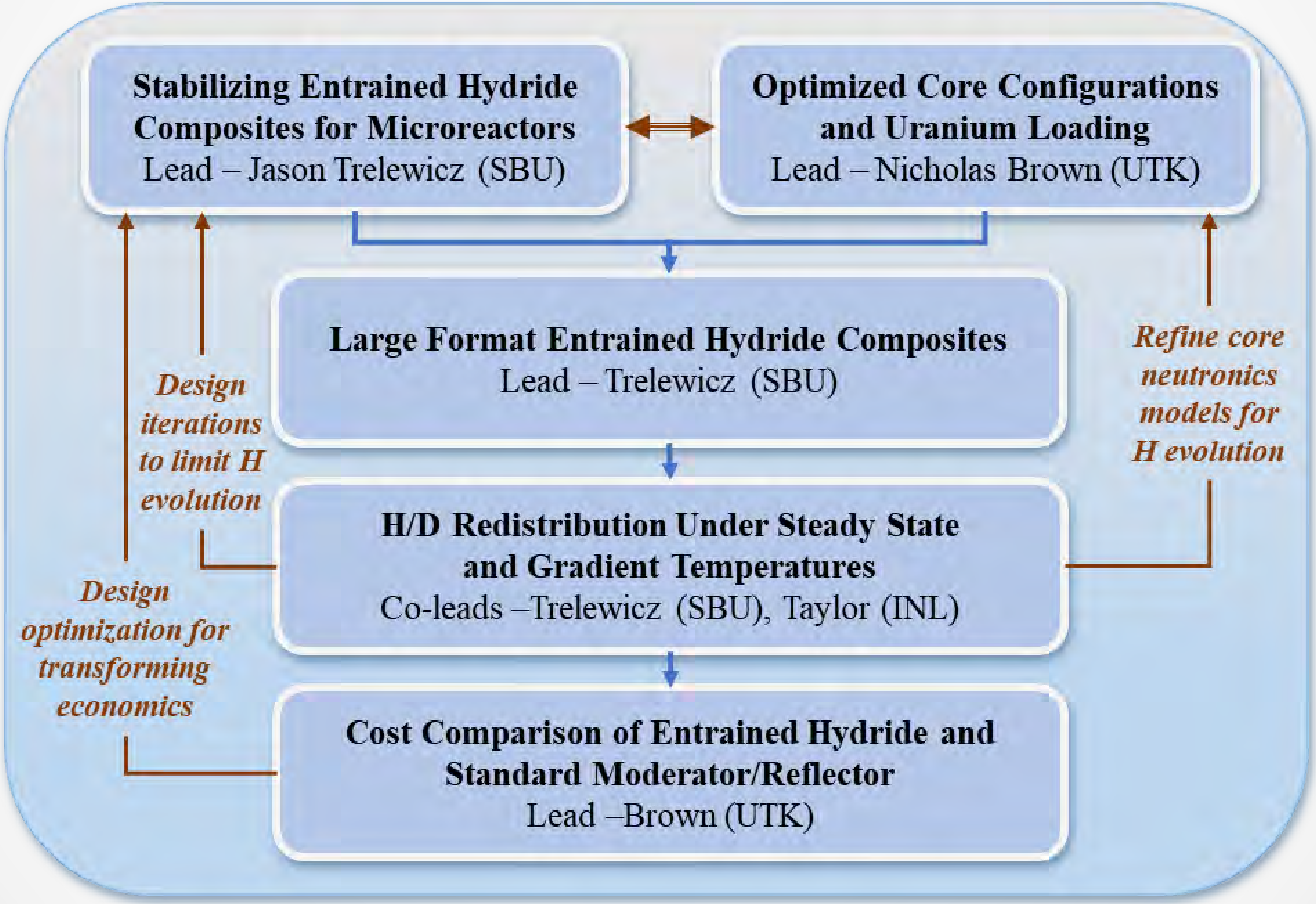


Figure 4: Core Critica



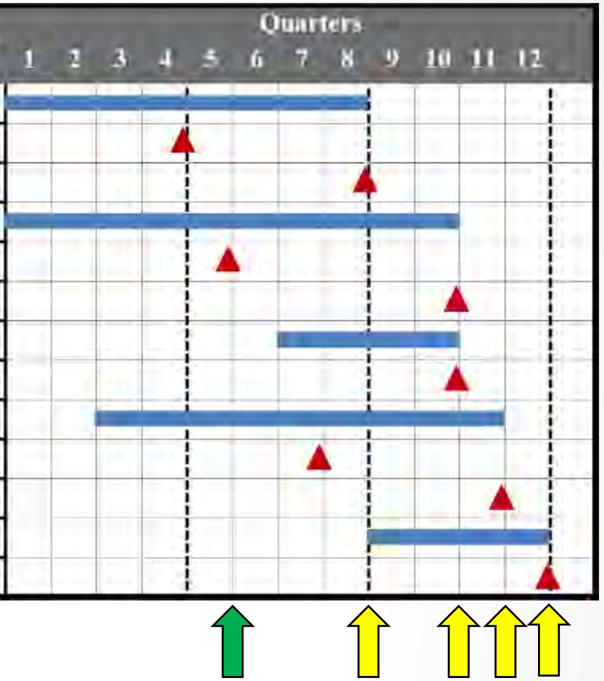


Task structure and technical feedback loops



Project schedule and milestones

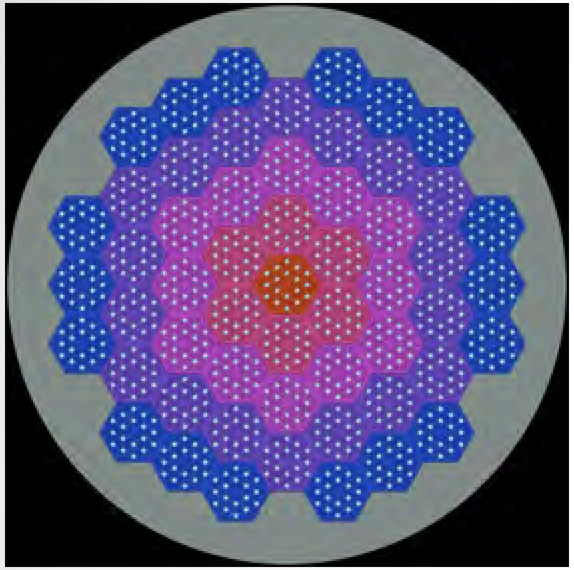
WBS	Task/Milestone Title	Start	End
Task 1a	**Microreactor-specific Entrained Hydride Development**	1	8
M1.1	Fabricate crack-free (ZrHx/YHx)-MgO composites	4	4
M1.2	Demonstrate stability at 800°C through an encapsulation barrier	8	8
Task 1b	**Optimized Microreactor Core Configurations and U Loading**	1	10
M1.3	Annular spherical core designs with composite moderators	5	5
M1.4	Technical report on fuel cycle performance with composites	10	10
Task 2	**Large Format Entrained Hydride Composites**	7	10
M2.1	Technical report on scaling of the entrained hydride composites	10	10
Task 3	H redistribution under steady state and gradient temperatures	3	11
M2.1	Hydrogen migration model for MgO within BISON	7	7
M2.2	Technical report on hydrogen desorption and transport properties	11	11
Task 4	**Cost Comparison of Hydride and Standard Technologies**	9	12
M4.1	Economic impacts report on entrained hydride composites	12	12



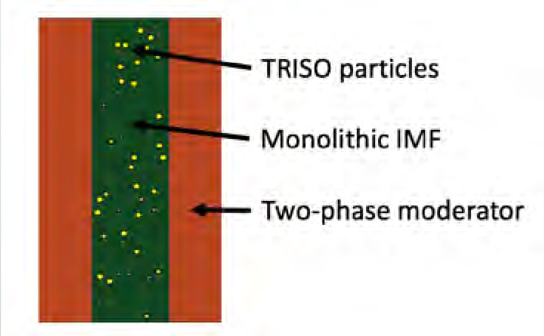
Milestones

1. Report on the fabrication of stabilized entrained hydride ceramic composites with hydride loading optimized based on the annular spherical core models and stability up to 800°C
2. Report on fuel cycle performance of the spherical cores optimized to exploit the enhanced neutron economy enabled by the hydride-entrained composite moderators and reflectors.
3. Report on hydrogen transport in the entrained hydride composites coupled with a hydrogen migration model for MgO and its impact on fuel cycle performance under transients.
4. Technical Report on Large Format Production of Entrained Hydride Composites

Initial cylindrical design (previously optimized)



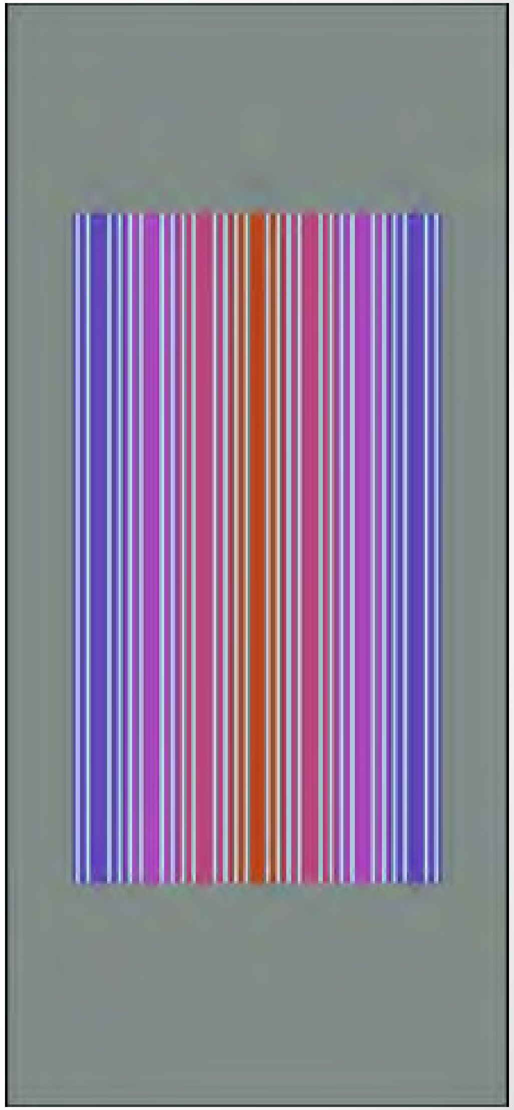
- 55 fuel blocks per layer
- 48 layers of fuel blocks
- 2640 fuel blocks
- Volume = 1.01*107[cm3]



- No coolant channels in reflector to simplify conversion to sphere
- Calculate the sphere radius:

$$V_c = \pi r^2 h \quad R_c = 90[cm] \quad H_c = 395.5[cm]$$
$$V_s = \frac{4}{3}\pi r^3 \quad R_s = ?$$
$$V_s = V_c$$
$$\frac{4}{3}\pi R_s^3 = \pi R_c^2 H_c$$
$$\frac{4}{3} R_s^3 = R_c^2 H_c$$
$$R_s^3 = \frac{3}{4} R_c^2 H_c$$
$$R_s = \sqrt[3]{\frac{3}{4} R_c^2 H_c}$$
$$R_s = \sqrt[3]{\frac{3}{4} 90^2 (395.5)} = 133.936[cm]$$

- Fill with the same number of fuel blocks

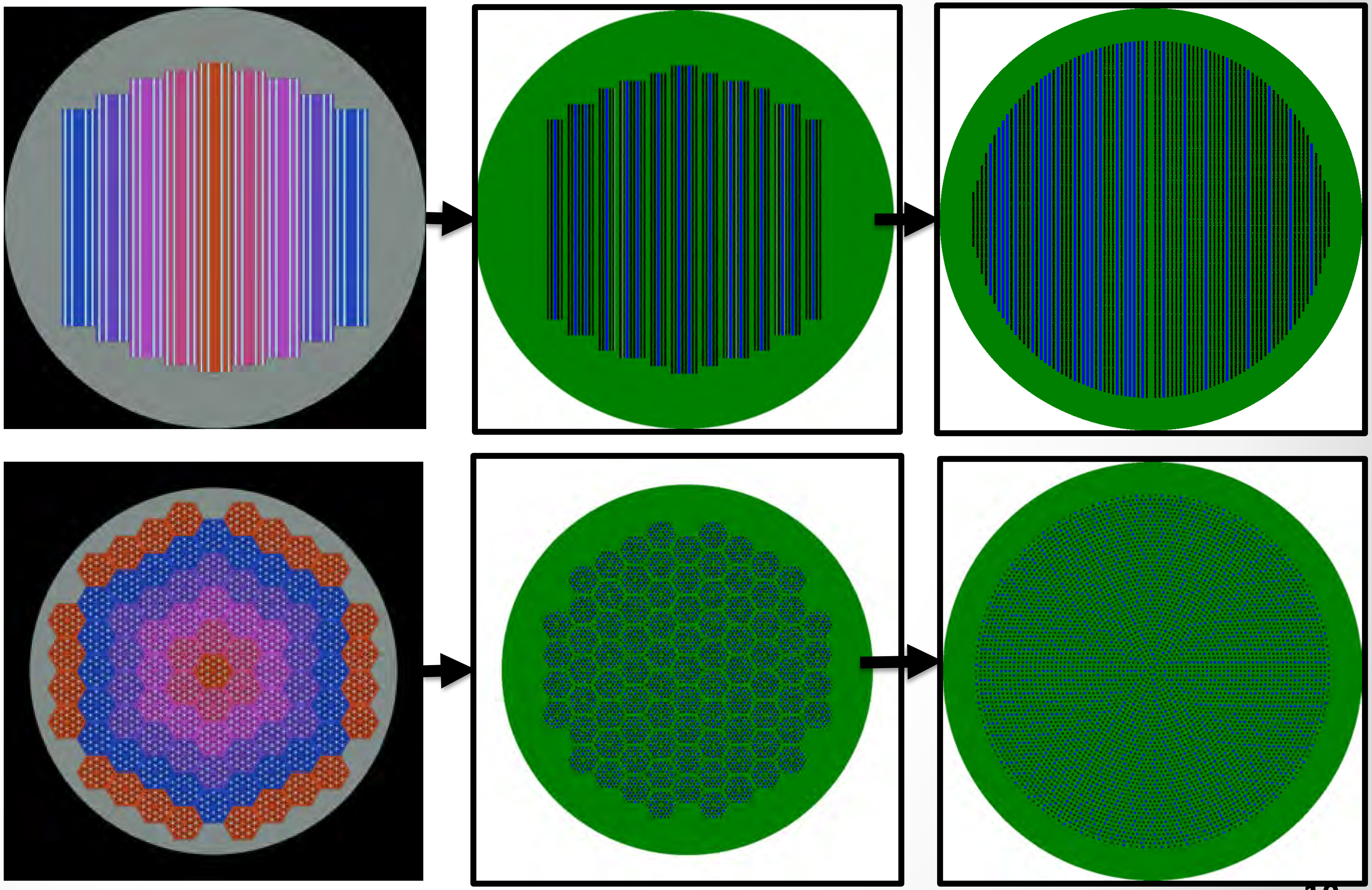


Spherical design refinement holding core volume constant

- Lower probability of neutron leakage due to lower surface area to volume
- Reduced neutron leakage increases discharge burnup

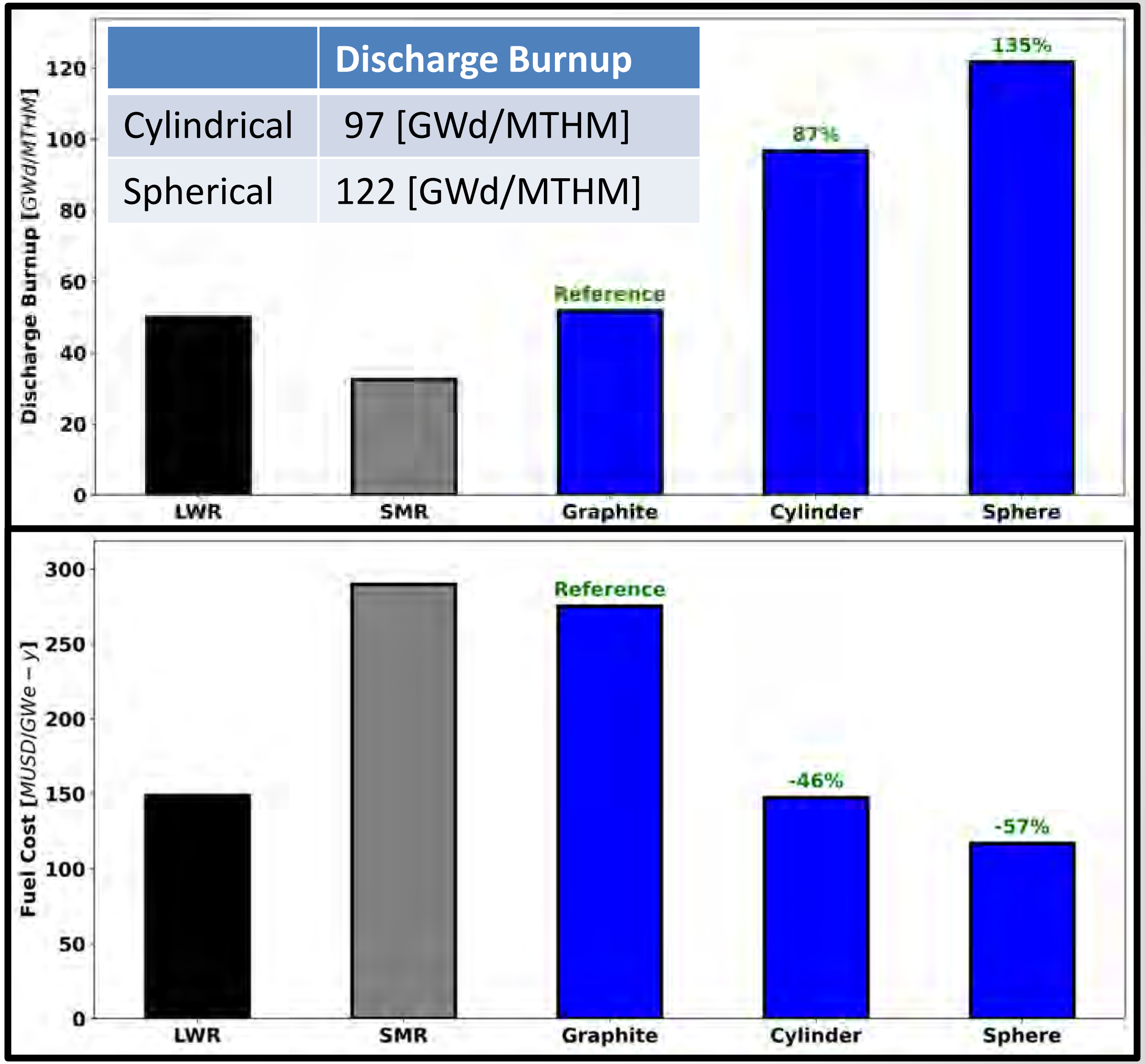
$$K_{eff} = \eta \epsilon p f P_f P_t$$

η = reproduction factor
ϵ = fast fission factor
p = resonance escape probability
f = thermal utilization factor
P_f = Fast Non-leakage Probability
P_t = Thermal Non-leakage Probability



Performance of the optimized spherical microreactor design

- Identical volumes with MgO-ZrH moderated moderators
- Sphere produces a **<u>22% increase in burnup</u>** from a geometry change
- Compared to a cylindrical graphite mHTGR refence the spherical design has a 135% increase in discharge burnup
- Spherical designs reduce fuel costs and mass of SNF by 57% compared to graphite reference

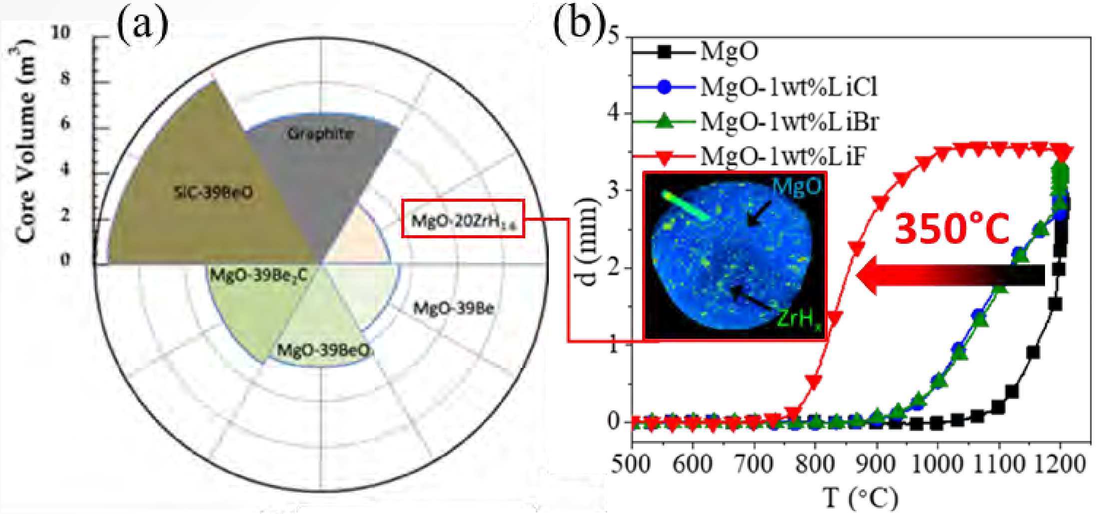


	Discharge Burnup
Cylindrical	97 [GWd/MTHM]
Spherical	122 [GWd/MTHM]

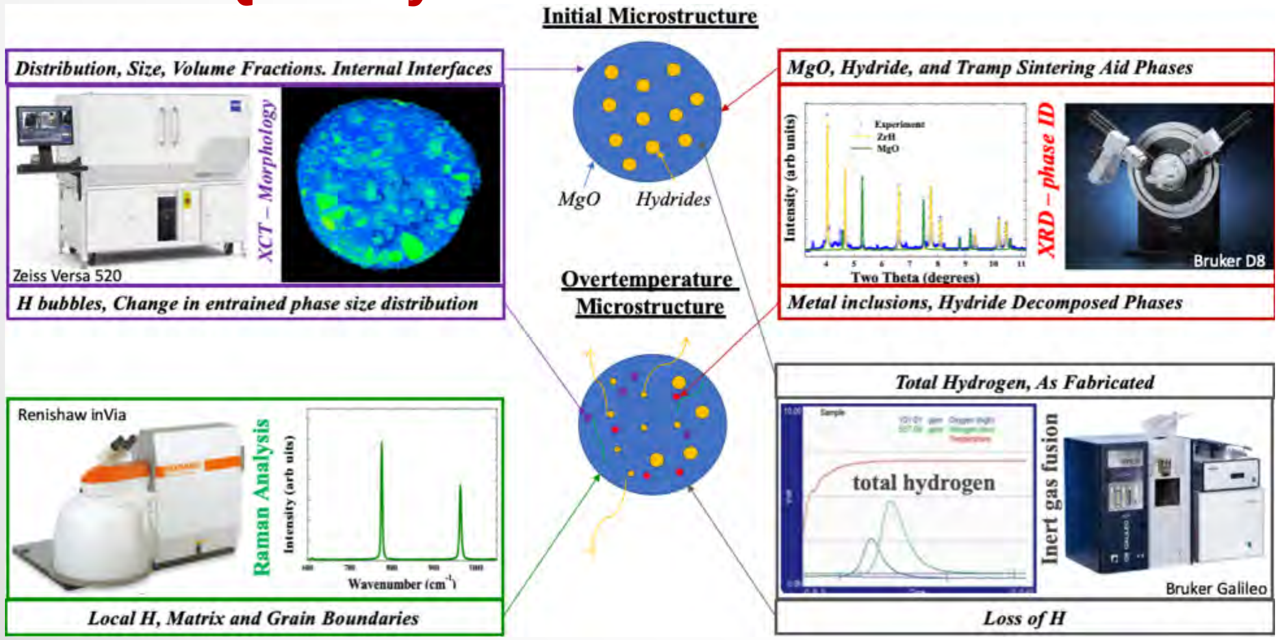
Composite moderator development

Modeling informed composite fabrication

Cladding implementation

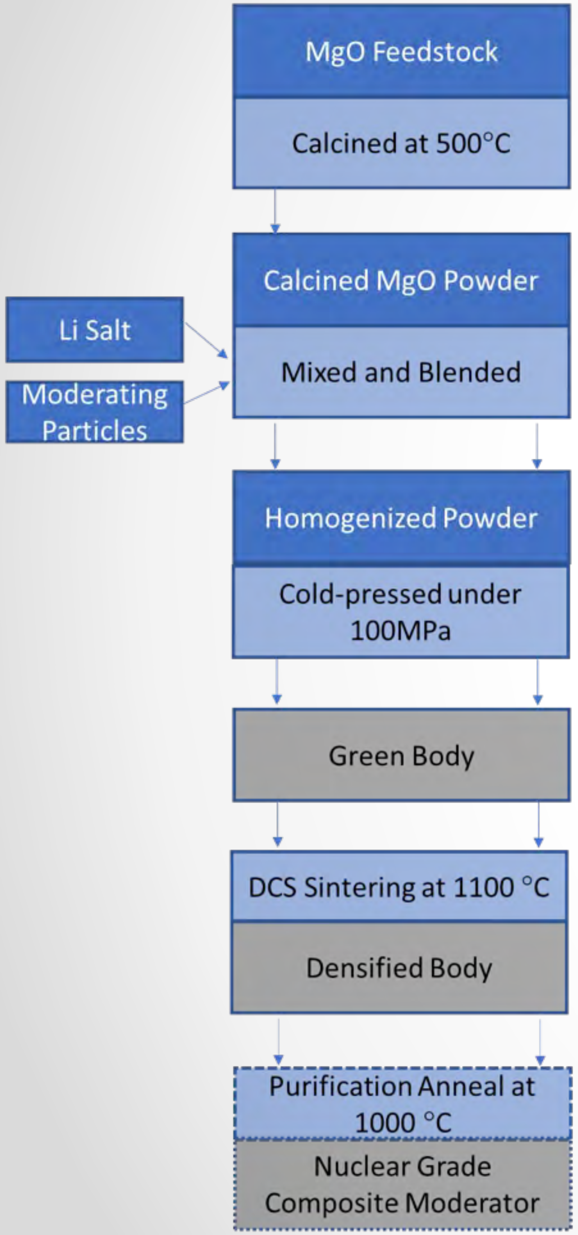


Quantify structural characteristics → Thermal stability

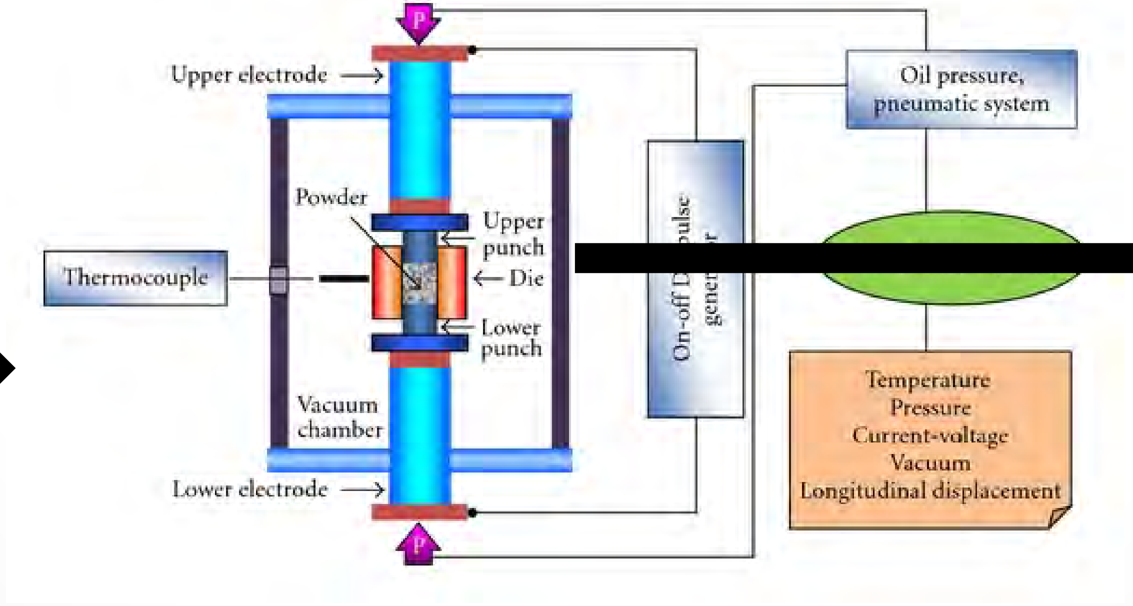


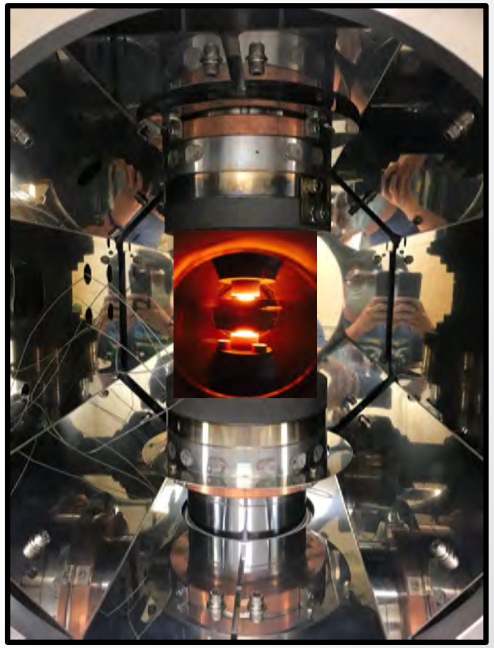
Hydride stability and retention

Field assisted sintering (short thermal excursions)

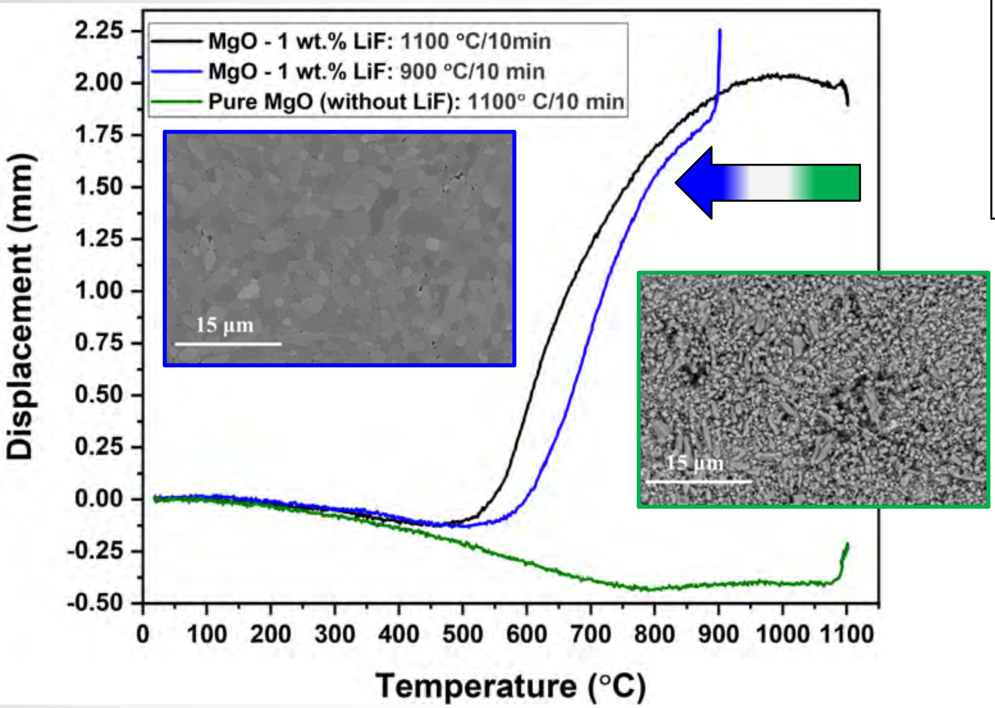


Sintering conditions:	**Temperature profiles:**
Sintering pressure: 10-50 MPa	Sintering temperature: 800 - 1200 °C
Graphite die diameter: 25 mm	Heating rate: 50 °C/min
Atmosphere: Vacuum	Cooling rate: 25 °C/min

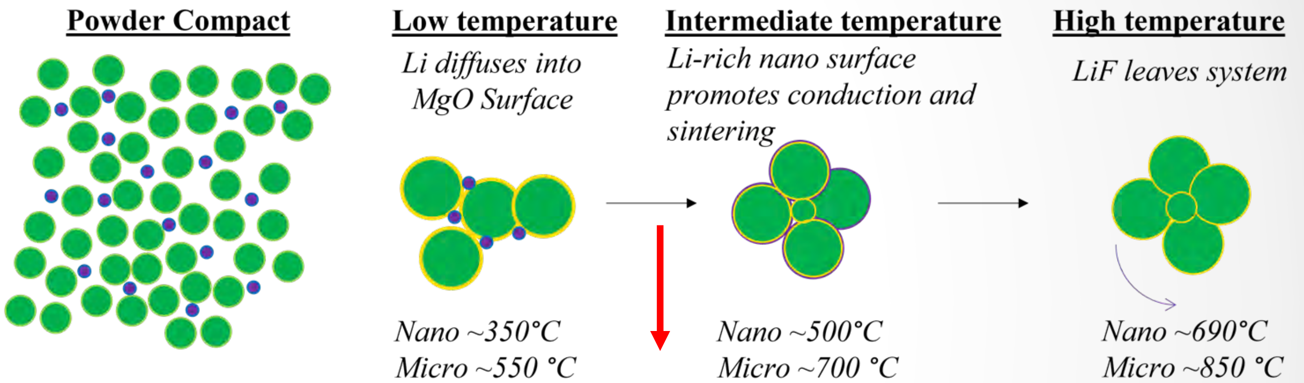




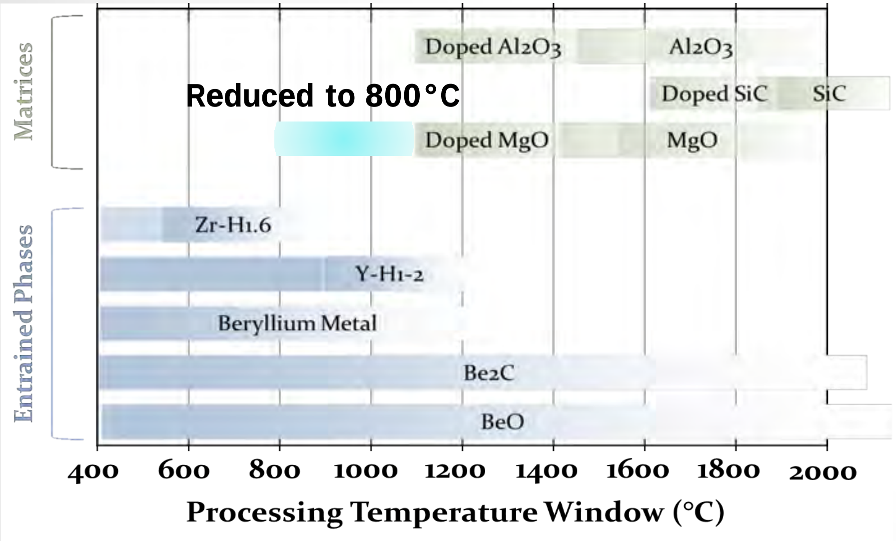
Enabling hydride composites through MgO sintering technology

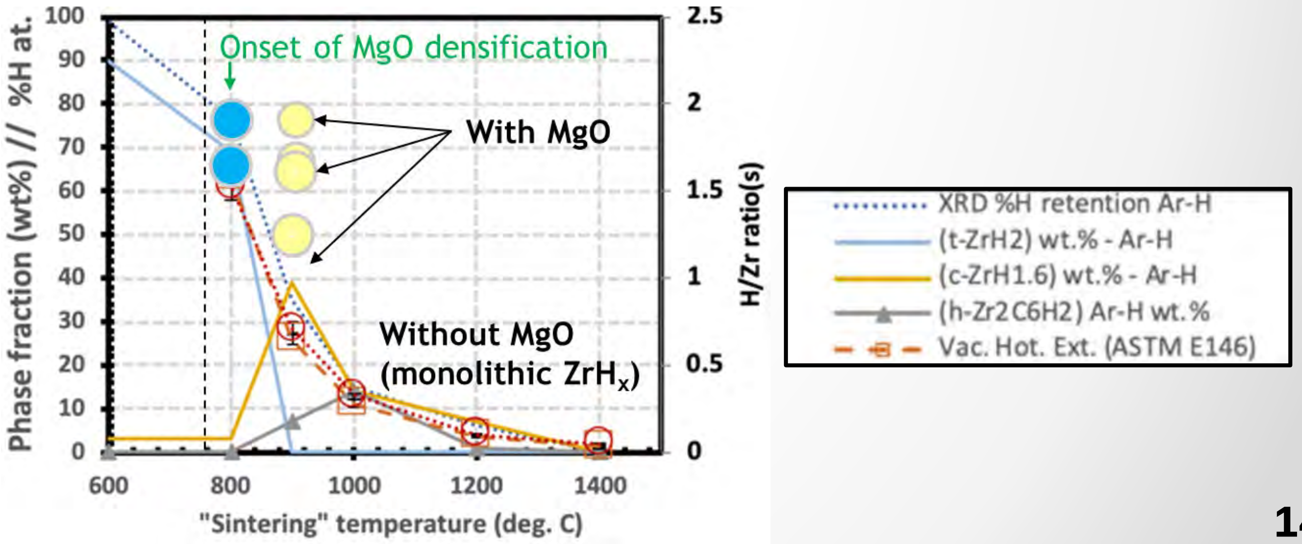


- Lowering of **onset temperature for sintering by ~500 °C** (w.r.t pure MgO) in presence of LiF as a sintering aid
- **~99% densification achieved at 900 °C**



Mg^{2+} vs. Li^{1+} => charge balance requires oxygen vacancies





Systematic variation in key processing parameters for MgO-ZrH_x

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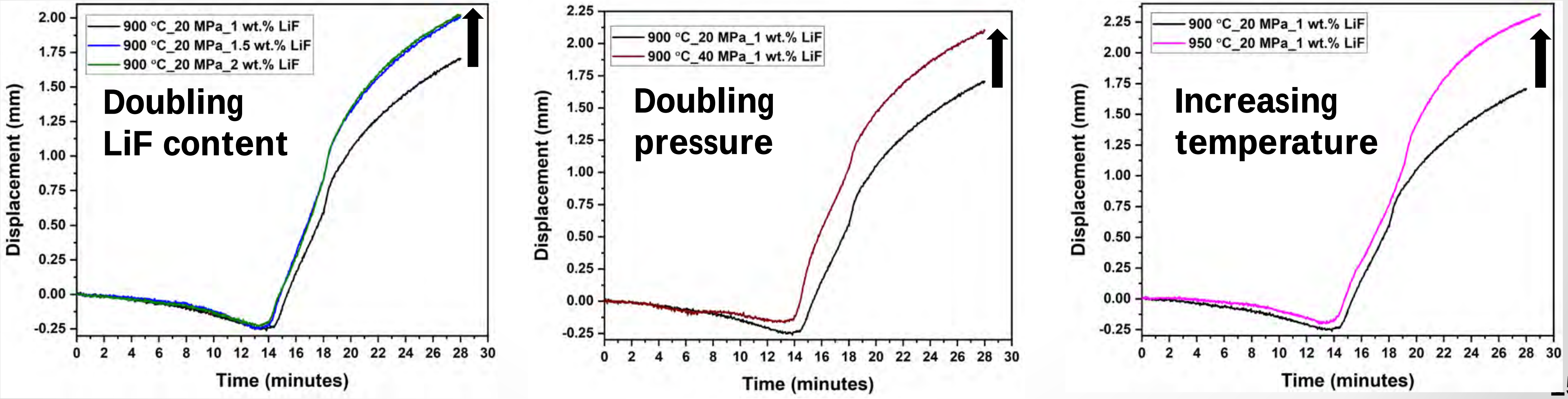
Parameters considered

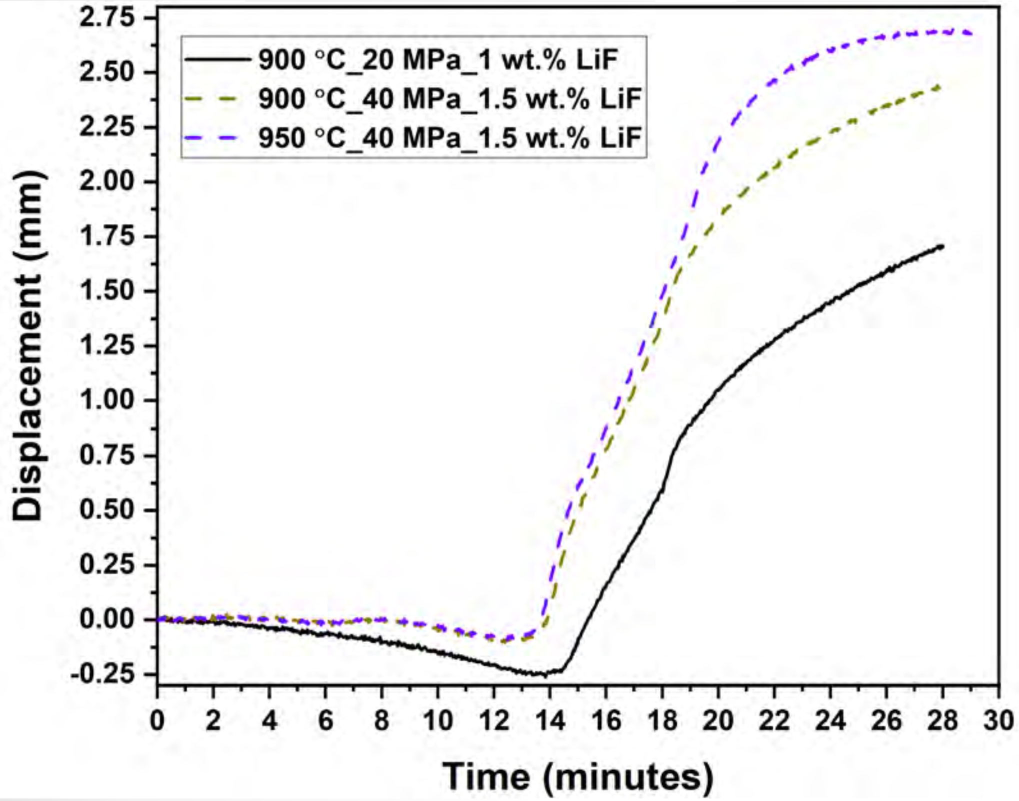
- LiF content
- Sintering pressure
- Sintering temperature

➔ *Use same ramp rates, and constant 10 min hold*

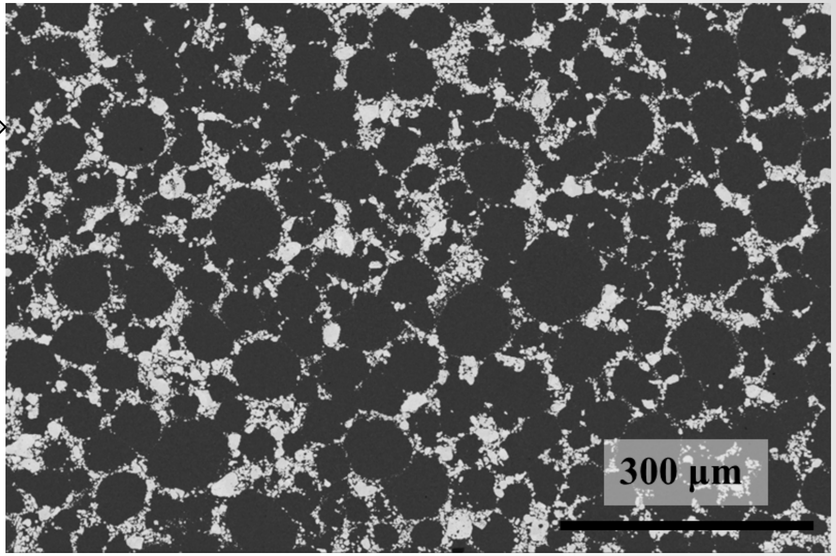
Sintering temperature (°C)	LiF Content Wt.%	Sintering pressure (MPa)	Density (g/cm^3)	Relative density (% of ρ_{th} = 3.98)
900	1.0	20	3.29	82.66
900	1.5	20	3.40	85.42
900	2.0	20	3.44	86.42
900	1.0	40	3.51	88.19
950	1.0	20	3.70	92.96



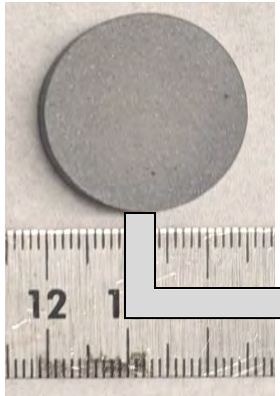
Optimized MgO-ZrH_x composites

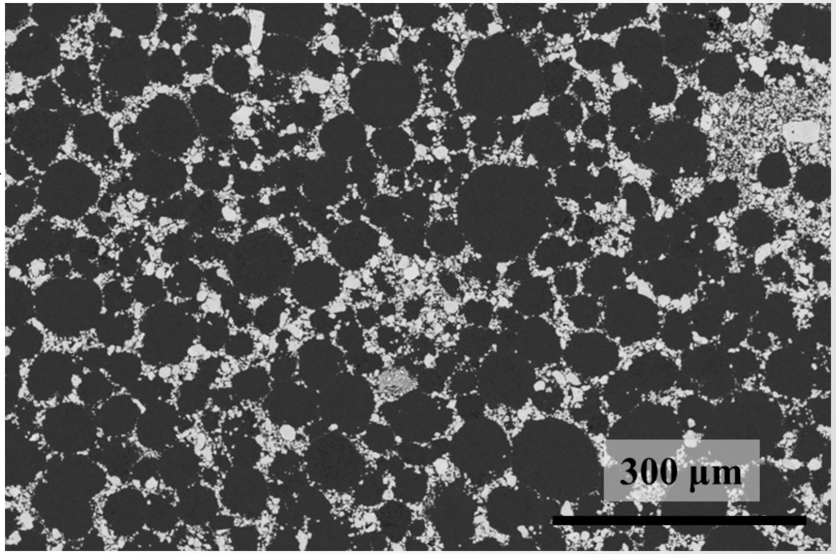


950°C



900°C





Sintering temperature (°C)	Wt.% LiF (w.r.t. MgO)	Pressure (MPa)	Density (g/cm^3)	Relative Density (%)
900	1.0	20	3.29	82.66
900	1.5	40	3.76	94.47
950	1.5	40	3.93	98.74

Hydrogen migration model in MgO

Solid Solution

c_{SS} Concentration gradient (Fick's Law)

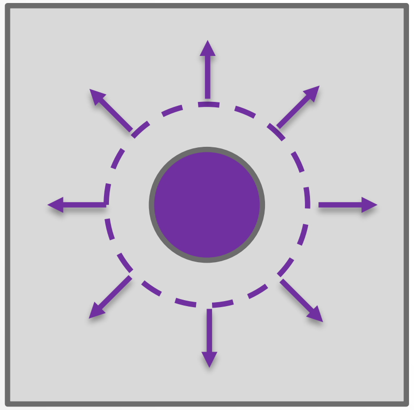
T Temperature gradient (Soret Effect)

Heat of transport

$$J_{Tot} = J_{Fick} + J_{Soret}$$
$$= -\boldsymbol{D_H}\left(\nabla C_{SS} + \frac{C_{SS}\boldsymbol{Q}^*}{RT^2}\nabla T\right)$$

H interdiffusion coefficient

Hydrides



Kinetic Parameters — Solubility Limit

$$\frac{\partial C_{SS}}{\partial t} = \begin{cases} -K_D(C_{SS} - TSS_D), & C_{SS} < TSS_D \quad \text{Dissolution} \\ -K_G(C_{tot} - TSS_D)p(1-x)(-ln(1-x))^{1-1/p}, & TSS_D < c_{SS} < TSS_P \quad \text{Growth} \\ -K_N(C_{SS} - TSS_P), & TSS_P < C_{SS} \quad \text{Nucleation} \end{cases}$$

Super-solubility Limit

$$x = \frac{C_{tot} - C_{SS}}{C_{tot} - TSS_D}$$

Passelaigue, F., Simon, P. C. A., & Motta, A. T. (2022). Predicting the hydride rim by improving the solubility limits in the Hydride Nucleation-Growth-Dissolution (HNGD) model. *Journal of Nuclear Materials*, *558*, 153363.

Key Assumptions and required inputs

- Material properties are uniform, isotropic, and time-independent (no microstructural effects)
- Kinetic factors are independent of the extent of transformation
- For first-order model, hydride nucleation and growth are ignored (dominated by dissolution)

Symbol	Parameter	Method
D_H	H Interdiffusion Coeff	Infrared Absorption
TSS_D	Solubility Limit	Differential scanning Calorimetry
Q^*	Heat of Transport	Measurement of H profiles under ∇T
K_D	Dissolution rate constant	Differential scanning calorimetry
k_{mob}	Mobility-limited growth constant	
k_{th}	Reaction-limited growth constant	
TSS_P	Supersolubility limit	
k_N	Nucleation kinetic parameter	

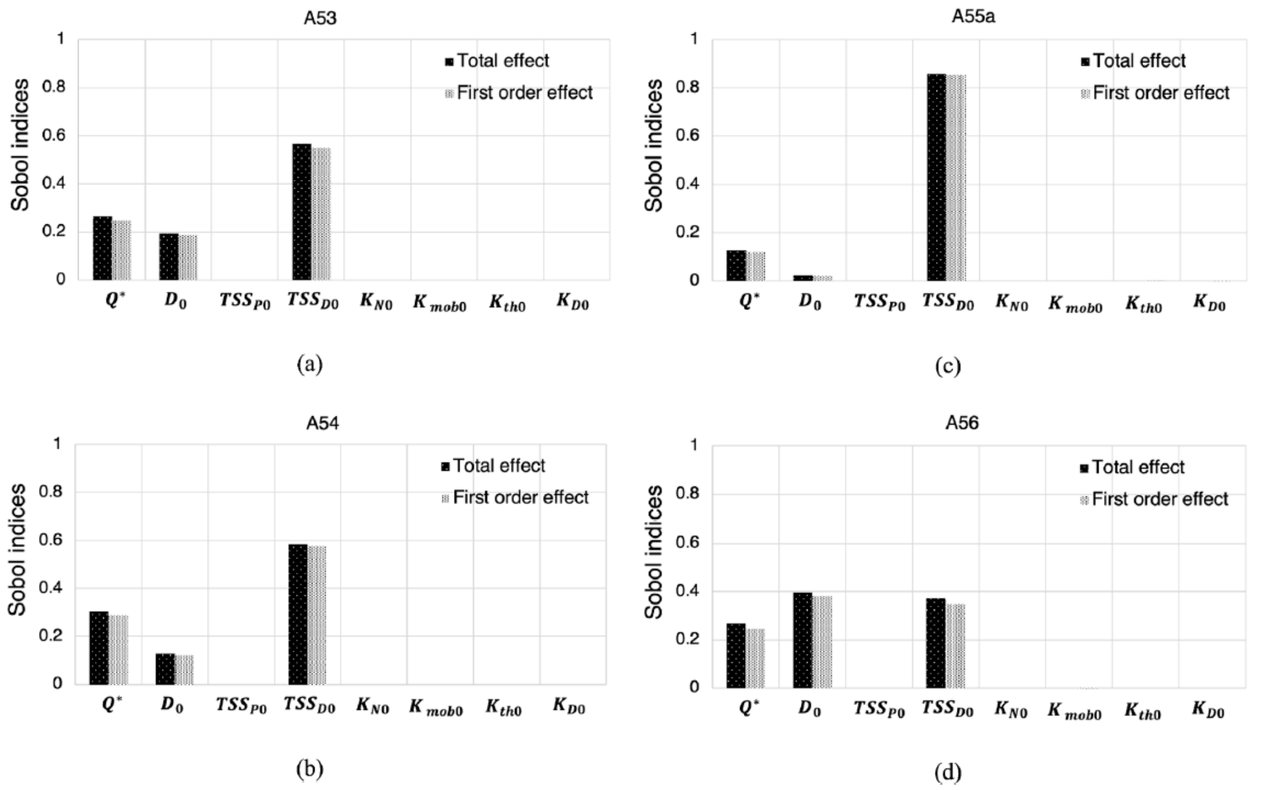
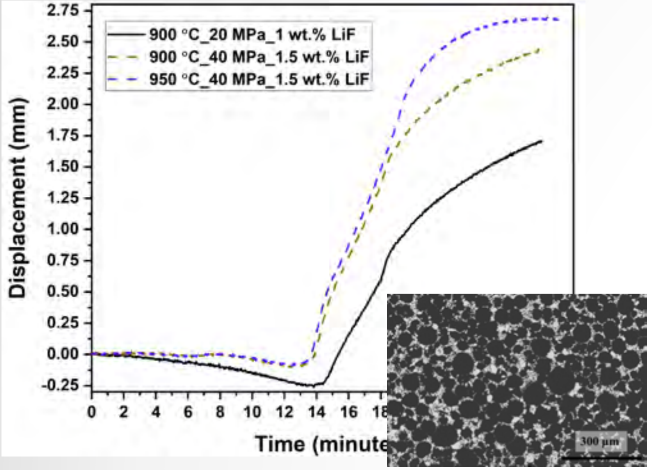
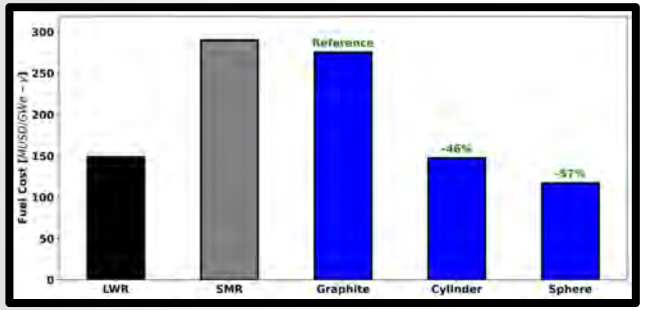


Fig. 11. Sobol indices of input parameters computed from RMSE for asymmetric cases: (a) specimen A53, (b) specimen A54, (c) specimen A55a, (d) specimen A56.

Seo, S. B., Duchnowski, E. M., Motta, A. T., Kammenzind, B. F., & Brown, N. R. (2022). Sensitivity analysis for characterizing the impact of HNGD model on the prediction of hydrogen redistribution in Zircaloy cladding using BISON code. *Nuclear Engineering and Design*, *393*, 111813.

Project status and looking forward





Next Steps

- Synthesize samples for thermal desorption spectroscopy (TDS) and hydrogen permeation experiments. (SBU)
- Quantify microstructures and hydride phase fractions in optimized samples using X-ray tomography and diffraction. (SBU)
- Perform TDS and permeation experiments. (INL)
- Determine model parameters using the outlined methods (SBU)
- Investigate encapsulation methods to further expand relevant operating temperature windows. (SBU)
- Outline moderator hydride loading using the prismatic spherical design and create pebble-bed spherical reactor design. (UTK)

Products

- First publication accepted – R. Altamimi, D. Doyle, J.R. Trelewicz, N.R. Brown, “Equilibrium Core Model for Micro Pebble-Bed Reactors Using OpenMC”, Nuclear Science and Technology, 2025
- Publication on sintering mechanism finalized and to be submitted April 2025
- Publication on process optimization in preparation

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