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National Laboratory

Bridging Thermal Scattering Law Data Gaps for Novel Moderators in Advanced Reactors

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Nuclear Data Group

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U.S. DEPARTMENT OF ENERGY

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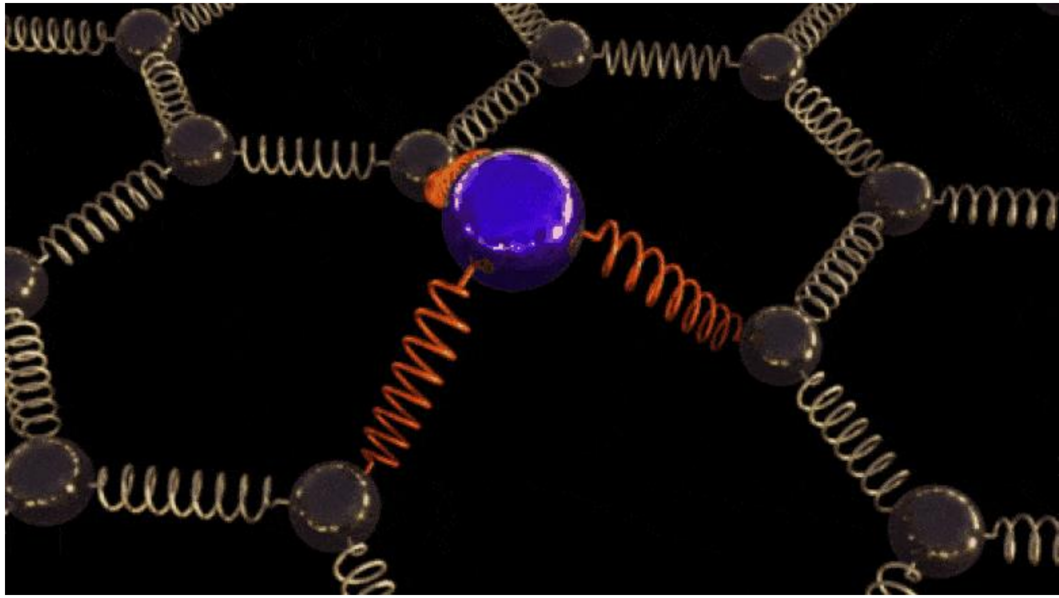
Outline

- Thermal Neutrons
- Summary of HALEU ARDP characteristics
- Neutron moderators' status
  - High Temperature Thermal Scattering Law (TSL) DNCSH Neutron Scattering Experiments
  - Critical DNCSH Benchmark Experiments
- Thermal Scattering Law Sensitivity and Uncertainty Status
- Potential Avenues

Thermal Neutrons

- Thermal neutrons have wavelengths (~Å) comparable to the separation distances of atoms in solids.
- Hence, the thermal motion of atoms or molecules in the scattering medium can no longer be ignored
- Thermal neutron scattering law (TSL) describes the neutron scattering intensity as a function of energy and momentum transfer between the thermal neutron and the scattering medium



Summary of HALEU ARDP characteristics

Lead	Reactor name	Reactor type	Neutron spectrum	Fuel type	Power	Enrichment (wt% ^{235}U)	Moderator	Reflector	Coolant
TerraPower	Natrium	SFR	Fast	Sodium-bonded metallic alloy U-10Zr Pins	345 Mwe	19.75	N/A	–	Sodium
X-energy	**Xe-100**	Pebble Bed HTGR	**Thermal**	UCO TRISO spherical compacts	**80 Mwe**	15.5	**Graphite**	**Graphite**	Helium
Kairos Power	**KP-FHR**	Pebble Bed FHR	**Thermal**	UCO TRISO annular spherical compacts with low-density graphite cores	**140 MWe**	19.55	**Pyrolytic graphite, FLiBe**	**Graphite**	**FLiBe**
Westinghouse Nuclear	**eVinci**	Heat-pipe Microreactor	**Thermal**	UCO TRISO cylindrical compacts	**5 MWe**	19.75	**Graphite**	**–**	Sodium Heat Pipes
Southern Company and TerraPower	MCFR	MSR	Fast	Dissolved uranium in salt ($NaCl\text{-}UCl_3$)	800 MWe	HALEU	N/A	–	Salt
BWXT	**BANR**	HTGR	**Thermal**	UN TRISO in SiC, carbon matrix compact, additively manufactured	**50 MWth**	19.75 (Baseline Design)	**Graphite**	**–**	Helium
ARC	ARC-100	SFR	Fast	Sodium-bonded U-10Zr pins	100 Mwe	20 Max.; 13.1 Avg.	N/A	Stainless steel	Sodium
GA-EMS	FMR	GFR	Fast	UO_2 pellets	44 Mwe	19.75	N/A	**Zr_3Si_2 and graphite**	Helium
MIT	**HC-HTGR**	HTGR	**Thermal**	TRISO compact	**~58 MWth**	**–**	**Graphite**	**–**	Helium

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Neutron moderators' status

Material	Available TSL ENDF Files	Differential XS Meas.	Integral XS Meas.	Benchmark* Experiments
Graphite	Yes	Yes	Yes	Yes
$ZrH_{1.6}$ & ZrH_2	Yes	Yes	Yes	Yes
YH_2	Yes	Yes	Yes	No
Be metal	Yes	Yes	Yes	No
BeO	Yes	No	Yes	No
MgO	Yes * *	Yes * * *	Yes	No
Be_2C	Yes	No	No	No
FLiBe	Yes	No	No	No
SiC	Yes	Yes * * *	Yes * * *	No
Zr_3Si_2	No	No	No	No

Fassino et al., “Current State of Benchmark Applicability for Commercial-Scale HALEU Fuel Transport,” ORNL/TM-2024/3248.

Al-Qasir et al., *Trans. ANS*, **130**, 750–753 (2024).

* Benchmark experiments involve fuel compositions ranging from 5 to 19.75 wt% enrichment of ^{235}U exhibiting a neutron flux of <0.625 eV (*International Handbook of Evaluated Reactor Physics Benchmark Experiments* [IRPhE]).

* * MgO TSL sub-library added recently to ENDF/B-VIII.1 as a neutron filter.

* * * Neutron scattering measurements were performed recently, not published yet.

High-temperature DNCSH neutron scattering experiments

UF6 transportation
10-20% enrichment gap
Non-fissile material validation
Fissile salts
✓ Graphite and advanced moderator nuclear data

- Two proposals have been awarded by DNCSH Experiment and Analysis Work Package (EAW) Call #1
  - State-of-the-art neutron scattering instruments will be used for neutron scattering measurements of differential and integral quantities.
  - Modern computational solid-state physics methods will be utilized to study atomic vibrations as a function of temperature

Material	Available TSL ENDF files	Differential XS measurement	Integral XS measurement	Benchmark experiments
Graphite	Yes	Yes	Yes	Yes
BeO	Yes	No	Yes	No
MgO	Yes	Yes	Yes	No
Be_2C	Yes	No	No	No
FLiBe	Yes	No	No	No
SiC	Yes	Yes	Yes	No
ZrC	No	Yes	Yes	No

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Critical benchmark DNCSH experiments

UF6 transportation
✓ 10-20% enrichment gap
Non-fissile material validation
Fissile salts
Graphite and advanced moderator nuclear data

- 14 proposals have been awarded by DNCSH EAW Call #1
- Of the 14 proposals, 6 were awarded for graphite, 3 for SiC, 1 for zirconium hydride, and 1 for beryllium metal

	Award	Moderator	Lead Lab	Partners
1	Benchmark of Historical Y-12 Critical Experiments with UF6 Cylinder Model 8A Containers	UF6, polyethylene, concrete	ORNL/LLNL	ORNL, CS Engineering, University of Tennessee
2	Evaluation of already performed critical experiments and design of new critical experiments with the new 19.75 wt% 235U enriched IPEN/MB-01 core for ICSBEP publication	Graphite, water, heavy water	ORNL	GE Vernova, IPEN (Brazil)
3	Evaluation of SLOWPOKE-2 Refuel Measurements	Beryllium metal	ORNL	Canadian Nuclear Laboratories (Canada)
4	Evaluation and BM Development of Reactor Critical Experiments of the RPI Reactor Critical Facility with Noteworthy Non-fissile SS Element Sensitivity	Water	ORNL	INL, Rensselaer Polytechnic Institute
5	Characterization of ISU's AGN-201 Reactor for Qualification as an ICSBEP Benchmark	Graphite	ORNL	GE Vernova, Idaho State University
6	Evaluation of Critical Configurations of the Missouri S&T Reactor	Water, graphite	ORNL	Missouri S&T
7	ZED-2 Measurements with In-Core Absorbers	Heavy water	ORNL	Canadian Nuclear Laboratories (Canada)
8	Critical Experiments Targeting Optimum Moderation Conditions	Water	PNNL	SNL, ORNL
9	PETALE benchmark	Water	LLNL	ORNL, EPFL, University of California-Berkeley
10	Benchmark Validation for Transportation of TRISO HALEU Fuel for Advanced Reactors	GRAPHITE, SiC from pebbles	INL	BWXT, Kairos, X-Energy, Radiant, Jfoster, U. Mich.
11	THETA: TRISO-form HALEU-fueled Experiment for Transport Applications	GRAPHITE, SiC from pebbles	LANL	Kairos Power
12	Thermal/Epithermal eXperiments (TEX) Additional Chlorine Configurations to Provide Validation for TerraPower's Molten Chloride Salt Fuel	Polyethylene	LLNL	LANL, TerraPower
13	eDeimos Experiments with Westinghouse for new HALEU Benchmarks	GRAPHITE, SiC from compacts and zirconium hydride	LANL	Westinghouse
14	HALEU Critical Experiments in Water Moderated UO2 Fuel Rod Lattices	Water	SNL	ORANO

Critical benchmark DNCSH experiments

	UF6 transportation
✓	10-20% enrichment gap
	Non-fissile material validation
	Fissile salts
	Graphite and advanced moderator nuclear data

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BeO	Yes	No	Yes	No	
MgO	Yes	Yes	Yes	No	
Be_2C	Yes	No	No	No	
FLiBe	Yes	No	No	No	
SiC	Yes	Yes	Yes	No	✓
Zr_3Si_2	No	No	No	No	

		Partners
1	Benchma	ORNL, CS Engineering, University of Tennessee
2	Eval expe	GE Vernova, IPEN (Brazil)
3		Canadian Nuclear Laboratories (Canada)
4	Evalua	INL, Rensselaer Polytechnic Institute
5	Charact	GE Vernova, Idaho State University
6		Missouri S&T
7		Canadian Nuclear Laboratories (Canada)
8		SNL, ORNL
9		ORNL, EPFL, University of California-Berkeley
10	Ber	BWXT, Kairos, X-Energy, Radiant, Jfoster, U. Mich.
11		Kairos Power
12	Thermal/	LANL, TerraPower
13		Westinghouse
14		ORANO

Thermal Scattering Law Sensitivity and Uncertainty Status

- Transport codes, like SCALE, calculate sensitivities of integral quantities to 1D cross sections $\sigma(E_i)$, but they do not address sensitivities to differential cross sections $\sigma\left(E_i \rightarrow E_f, \Omega_i \rightarrow \Omega_f\right)$.

- Covariance data are accessible for all neutron files but not for the 2D TSLs

- Presently, no published ENDF evaluations include covariance data for TSL or its corresponding scattering cross sections due to:
  - No agreed upon method for calculating covariances
  - No standardized format for storing & disseminating TSL covariances
  - Inability of transport codes to handle differential cross section covariances

- Recent efforts have focused on evaluating covariances in thermal neutron scattering for moderators like H_2O, D_2O, and graphite[1,2,3]

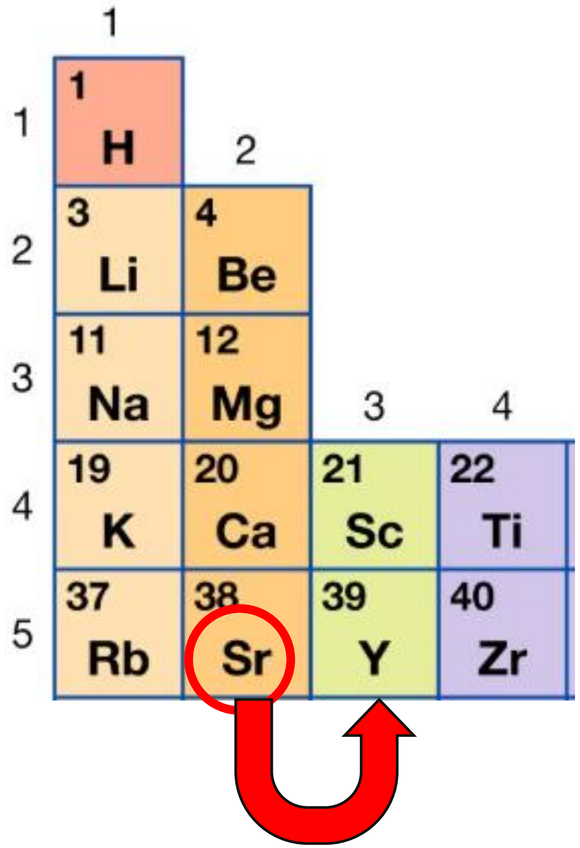
1. C. W. Chapman et al., "Methodology for Generating Covariance Data of Thermal Neutron Scattering Cross Sections," *Nucl. Sci. Eng.* **195**, 13 (2021).
2. J. P. Scotta et al., "Generation of the ^1H in H_2O Neutron Thermal Scattering Law Covariance Matrix of the CAB Model," *EPJ Nucl. Sci. Technol.* **4**, 32 (2018).
3. J. C. Holmes et al., "A Phonon-Based Covariance Methodology for ENDF S(α, β) and Thermal Neutron Inelastic Scattering Cross Sections," *Nucl. Sci. Eng.* **184**, 84 (2016).

Thermal Scattering Law Sensitivity and Uncertainty

- Three work packages have in initiated by DNCSH
  - Scoping study of sensitivities due to TSLs (Assess Impact of Unknown TSL on k, c_k)
  - Formatting and processing of eventual TSL covariance (TSL Uncertainty in ENDF/B for H_2O)
  - Code updating to use eventual TSL covariance (SCALE Inclusion of TSL Uncertainty in c_k)

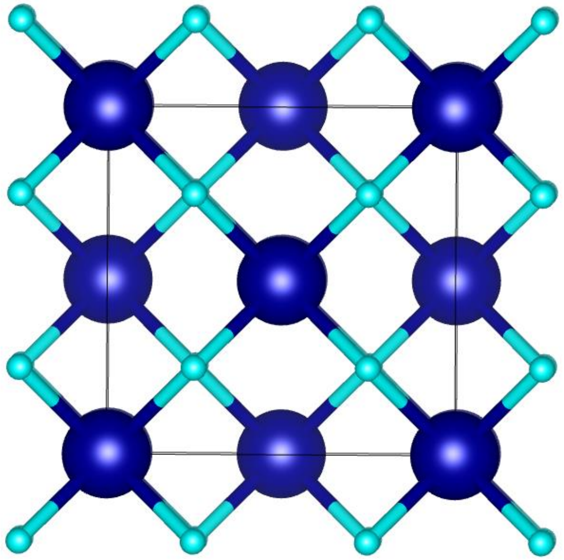
Potential Avenues

- **Tuning neutron moderators:** enhance neutron moderators through innovative material design at the microscopic (atomistic) and/or macroscopic (engineering) levels
  - ✓ **Doping**
  - ✓ **Two-phase composite materials**

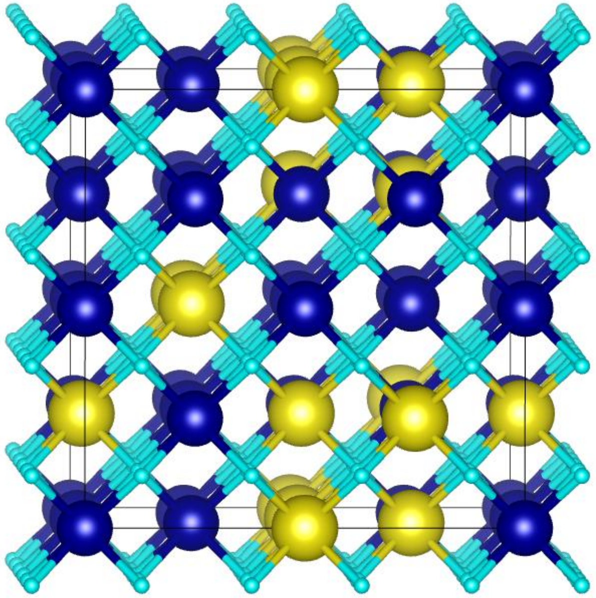


- Yttrium Hydride: High-temperature stability up to 800 ◦C

YH_2



$Y_{1-x}Sr_xH_2$

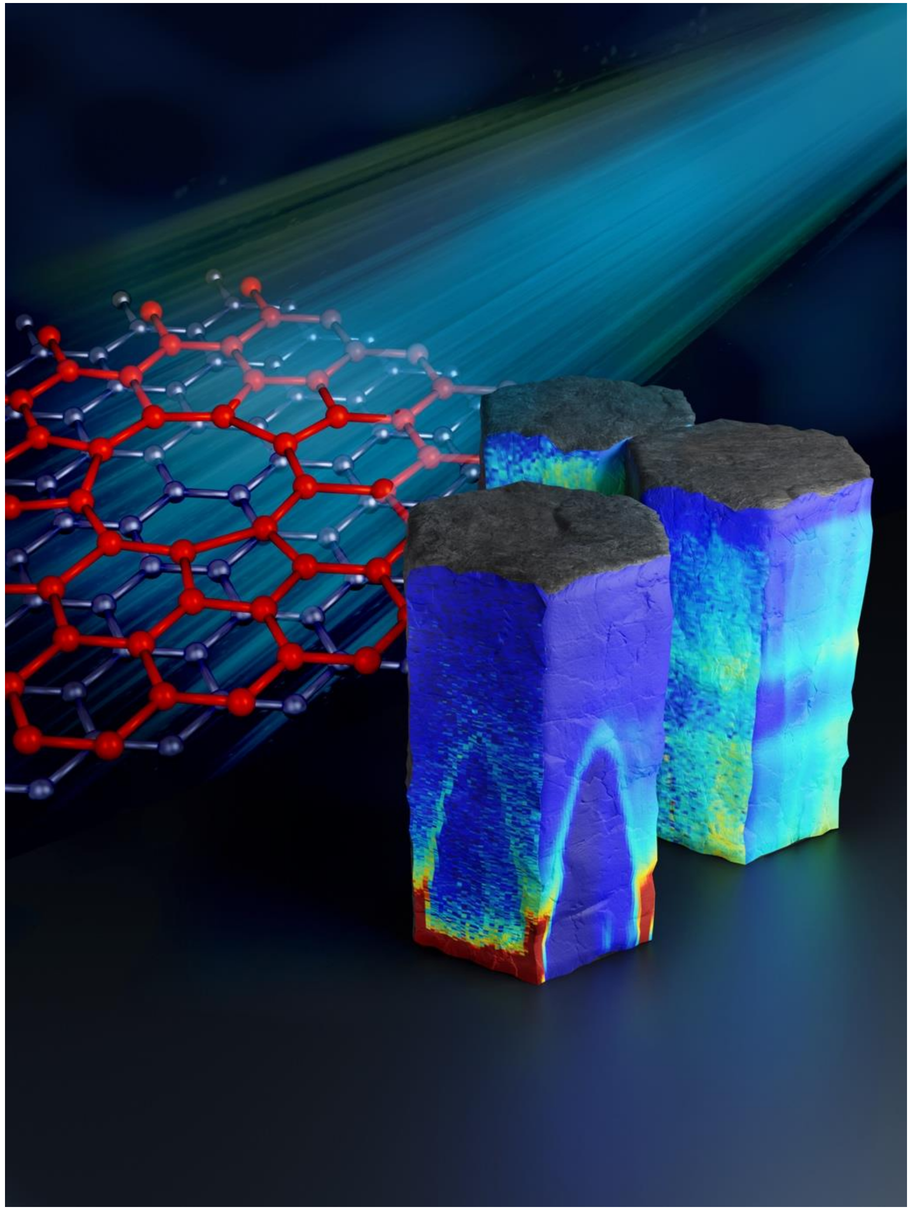


Isotope	Ab (%)	Scatt. XS (b)	Abs. XS (b)
^{88}Sr	82.58	6.42	0.058
Y	100	7.7	1.28

Acknowledgment

This work was performed under the framework of the DOE / US Nuclear Regulatory Commission (NRC) Collaboration for Criticality Safety Support for Commercial-scale HALEU (DNCSH) Fuel Cycles Project

Thank you



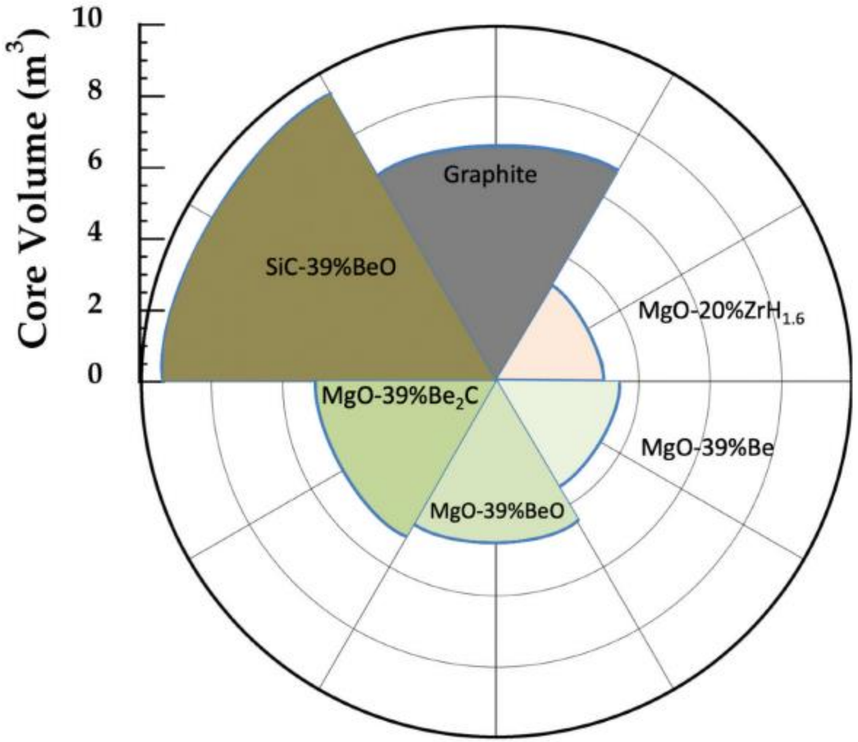
Materials science and engineering of neutron moderation

- Historically, core moderator and reflector materials consist of relatively simple compounds of a simple material type or simple composition (e.g., H_2O, D_2O, Be, BeO, Graphite, ZrH_2)
- Recently, compact thermal fission reactors are of increased interest because of their potential to lower construction cost, to enhance safety, and to facilitate portability to remote areas
- The compact nature of these cores requires good neutron economy, as well as preservation of other thermal, mechanical, and chemical properties, and more. How do we achieve this?

Materials engineering:
Two-phase composite moderators

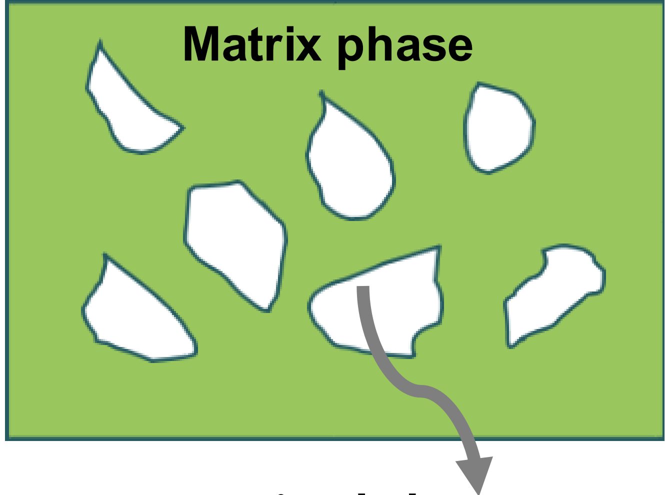
	Entrained phase	Matrix phase
Scattering	High	Fair
Absorption	Low	Low
Thermal conductivity	Fair	High
Radiation resistivity	Fair	Good
Mechanical stability	Fair	Good
Examples	Graphite, Be, BeO, **Be_2C**, **YH_{2-x}**, **ZrH_{2-x}**	MgO, SiC

Snead et al., *J. Asian Ceram. Soc.* **10**, 9 (2022).



Be_2C: reacts with moisture to form $Be(OH)_2$. However, as an entrained phase, it will not react

YH_{2-x}, ZrH_{2-x}: high-density matrix forms barriers that prevent hydrogen leakage

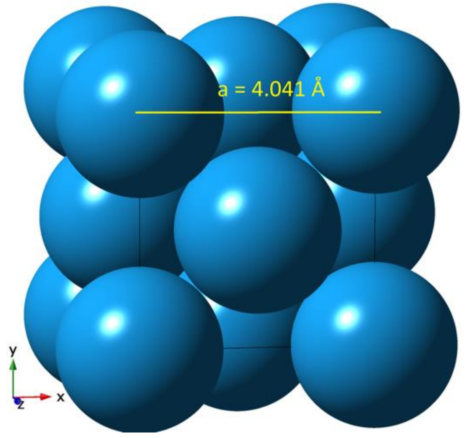


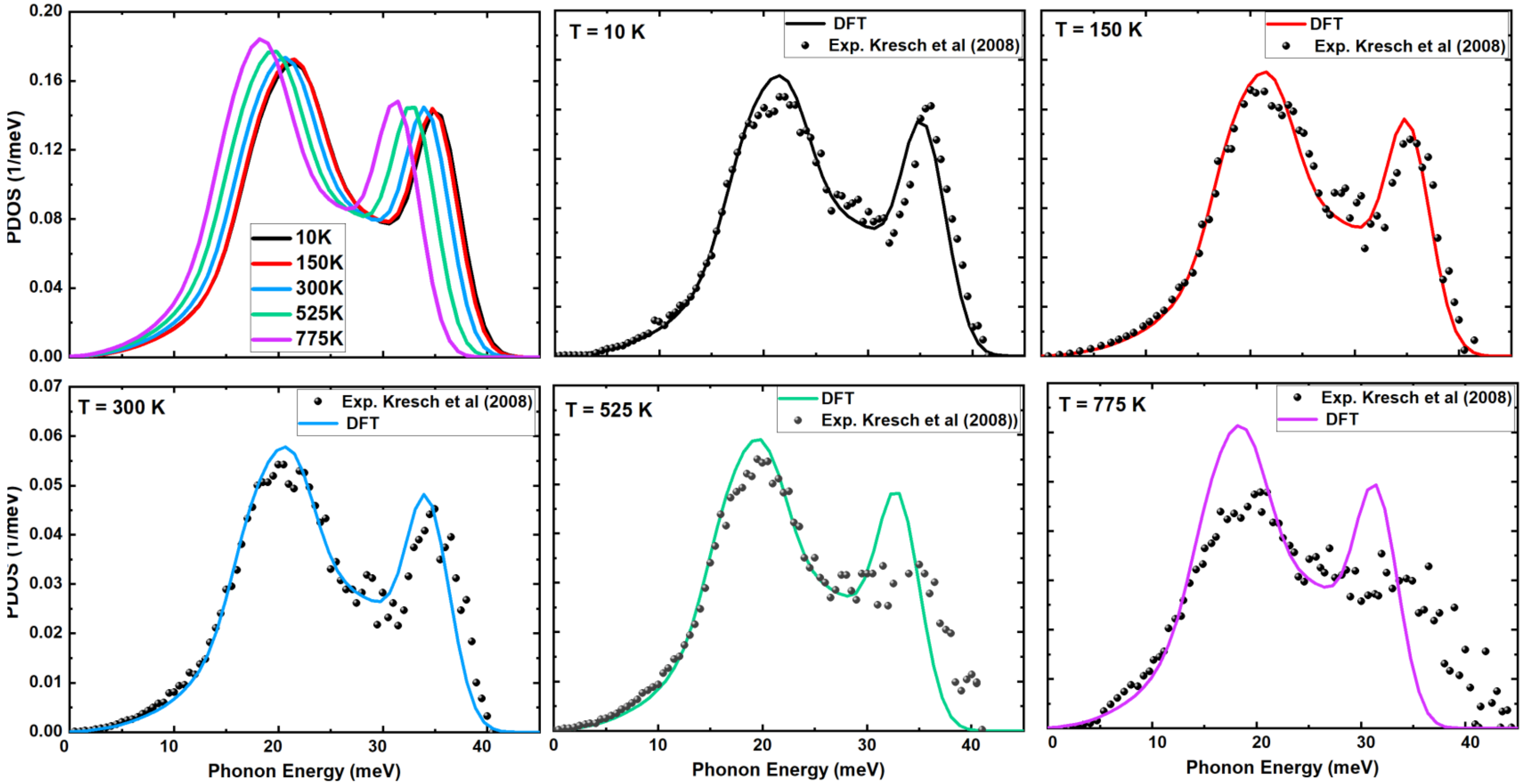
Entrained phase

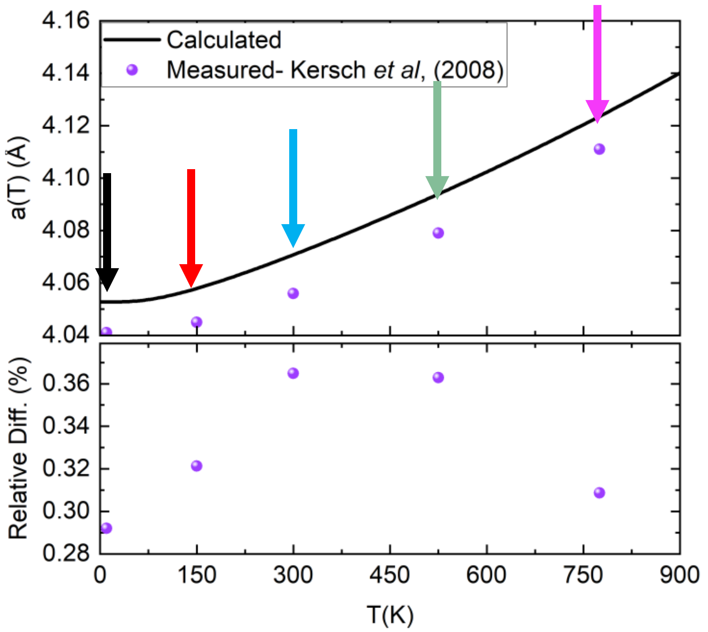
Entrained phase refers to a phase or component of a mixture that is carried along or transported by another medium or phase

MgO-based composite moderators can exhibit considerably smaller critical volumes compared to volumes of nuclear graphite

High-temperature TSL example: Aluminum







Kresch et al., Phys. Rev. B 77, 024301 (2008).

Inelastic scattering cross section

- Relative difference increases with increasing temperature
- σ(T) should be calculated using the PDOS corresponding to the same T