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Status update of ORNL ND11 task for FY23

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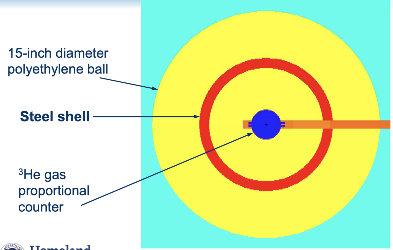
Outline

- Bonner spheres
- Polyethylene inelastic neutron scattering (INS) measurements
- Hydrated cement INS measurements
- Concrete INS measurements
- Hydrated cement and concrete transmission measurements

Bonner spheres

- Bonner sphere spectrometers have been used extensively in radiation protection practices to determine neutron spectral distributions around particle accelerators, nuclear power stations and other nuclear facilities, as well as in cosmic-ray neutron research for over two decades.

High-energy neutron detector



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NUSTL measurements

- NUSTL has measured the energy spectrum of cosmic-ray neutrons on:
- Airplanes
- Ground
- Ships

Components of NUSTL's new neutron spectrometer

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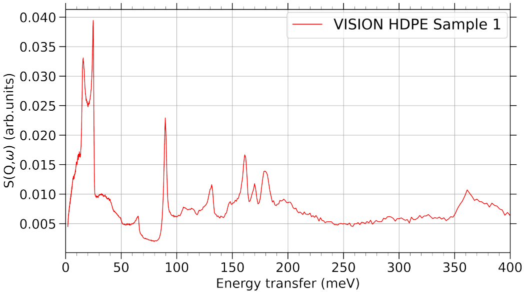
We can measure $S(\alpha, \beta)$

- INS indirect geometry spectrometers (VISION):



+ Measured quantity $S(Q, \omega, T)$ is directly related to $S(\alpha, \beta, T)$:

$$S(\alpha, \beta, T) = \frac{k_B T}{\hbar}\ exp\left(\frac{-\hbar\omega}{2k_B T}\right) S(Q, \omega, T) \quad (1)$$

where T is the temperature, and k_B is the Boltzmann constant.

+ This means that we **can directly measure $S(\alpha, \beta)$**, which is what we store in ENDF TSL files.
+ We can compare ENDF evaluations directly with these measurements by extracting $S(\alpha, \beta)$ along these trajectories and **applying well-known instrumental resolution**.
+ We do not have a neutronics model of the VISION instrument yet to account for some experimental effects, such as thickness for example.
+ These measurements are available to anyone through user proposal system at many facilities around the world (SNS at ORNL, NIST, ILL in France, ISIS UK, ESS Sweden, J-PARC in Japan).

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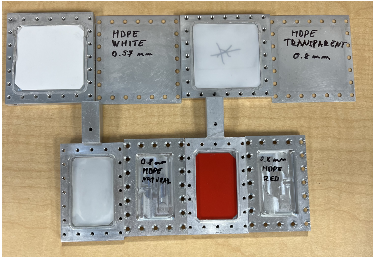
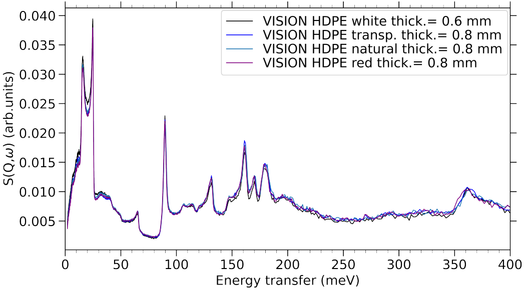
Polyethylene - HDPE $S(\alpha, \beta)$ measurements

Example: HDPE



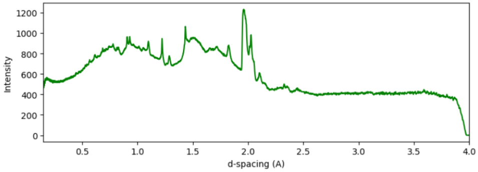
	Seller	Description
Sample 1	McMASTER-CARR	Moisture-Resistant HDPE Sheet, thickness 1/32", color white
Sample 2	McMASTER-CARR	Moisture-Resistant HDPE film, thickness 0.023", color opaque white
Sample 3	TAP Plastics	HDPE Matte/Matte Sheets, thickness 1/32", color natural
Sample 4	TAP Plastics	HDPE Matte/Matte Sheets, thickness 1/32", color red



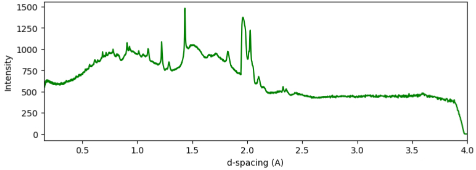
- HDPEs from different manufacturers, with different additives for color and properties, have similar shape of $S(\alpha, \beta)$.

Polyethylene - neutron diffraction measurements

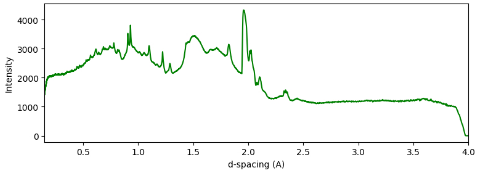
- Diffraction pattern HDPE red:



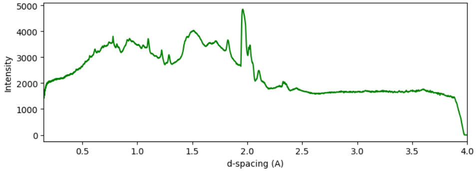
- Diffraction pattern HDPE natural:



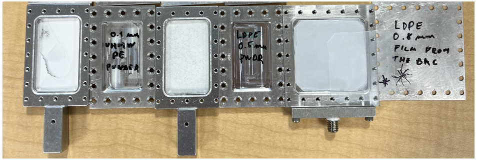
- Diffraction pattern HDPE white:

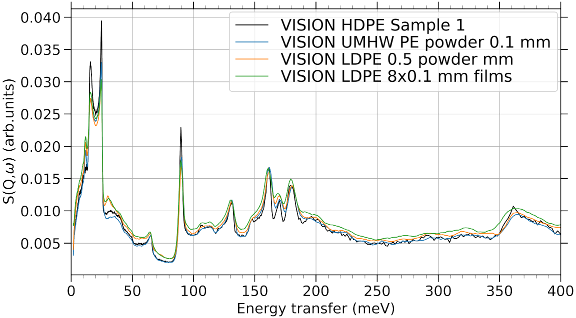


- Diffraction pattern HDPE transperent:



Polyethylene - LDPE and UHMW $S(\alpha, \beta)$ measurements

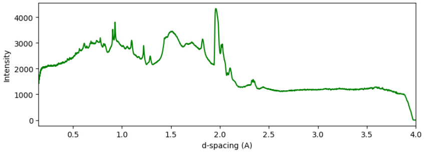




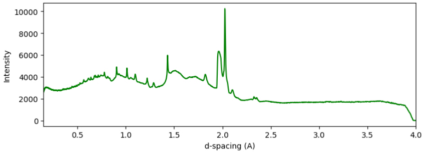
- LDPE and UHMW (ultra high molecular weight) PE completely structurally different from HDPE, have similar shape of $S(\alpha, \beta)$.

Polyethylene - neutron diffraction measurements

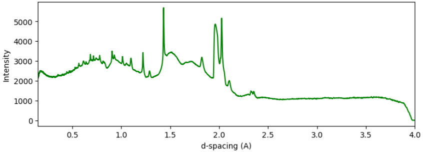
- Diffraction pattern HDPE white:



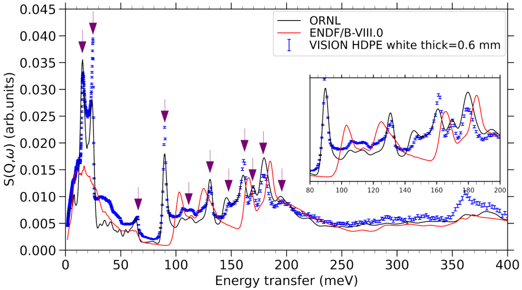
- Diffraction pattern LDPE:

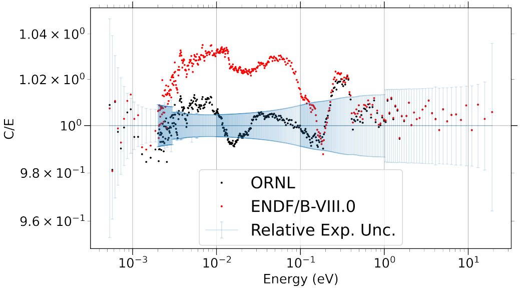


- Diffraction pattern UHMW PE:



Polyethylene - INS and transmission validation





TSL	VISION HDPE χ^2/d.o.f/d.o.f
ENDF/B-VIII.1.b3	187
ORNL	61.5

- ORNL evaluation has better agreement with the differential $S(\alpha, \beta)$ data!

Transmission exp.	ENDF/B-VIII.1.b3 χ^2/d.o.f	ORNL χ^2/d.o.f
RPI 2022	3.24E+5	2.33E+4
Lee 2020	2.3147E-2	2.3136E-2
Granada 1987	2.28E+5	1.77E+5
Herdade 1973	8.24e+05	1.68e+05

- ORNL evaluation has better agreement with the transmission data!

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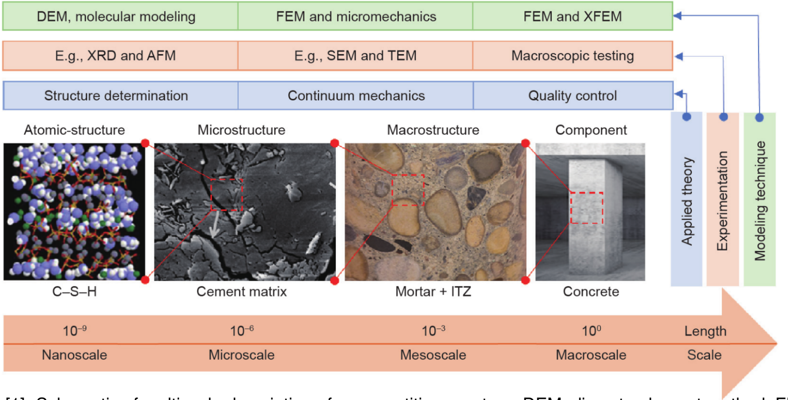
Hydrated cement and concrete challenges

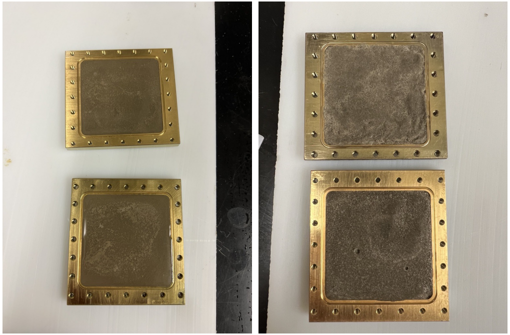


Reproduced from [1]. Schematic of multiscale description of a cementitious system. DEM: discrete element method; FEM: finite element method; XFEM: extended finite element method; XRD: X-ray diffraction; AFM: atomic force microscope; SEM: scanning electron microscopy; TEM: transmission electron microscopes; ITZ: interfacial transition zone.

- Unlike previous solid materials of interest to NCSP, there is no set structure for calcium-silicate-hydrate (CSH), which is 50%-65% by volume of hydrated cement paste, but we have been using different models available in the literature for modeling.

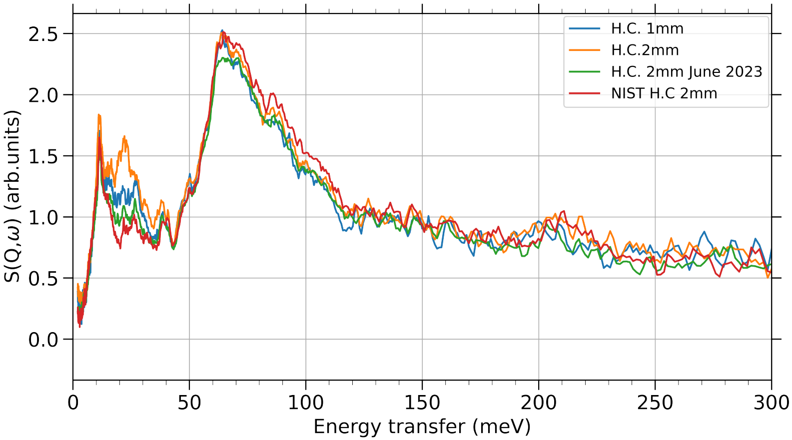
Hydrated cement and concrete measurements

- Hydrated cement composition: 50% water and 50% portland cement
- Concrete composition: 70% quartz(fine grain size for sample uniformity) and 30% hydrated cement (50% water and 50% portland cement mixture)
- INS measurements were performed in December 2022 (1 mm, 2mm, and 6 mm thickness samples, with portland cement off the shelf) and in June 2023 (2 mm sample thickness, with NIST standard portland cement). Samples were measured after 28 days of curing.
- Transmission measurements at RPI were performed in February 2023, same composition, 28 days curing period.



- **We want to test the assumption that the INS and transmission spectra of concrete are a linear combination of the spectra of hydrated cement and aggregates (in this case, quartz sand)**

Hydrated cement INS measurements



- Slight variation in the 10-35 meV range, but overall consistent shape of the measured $S(\alpha, \beta)$ spectra.

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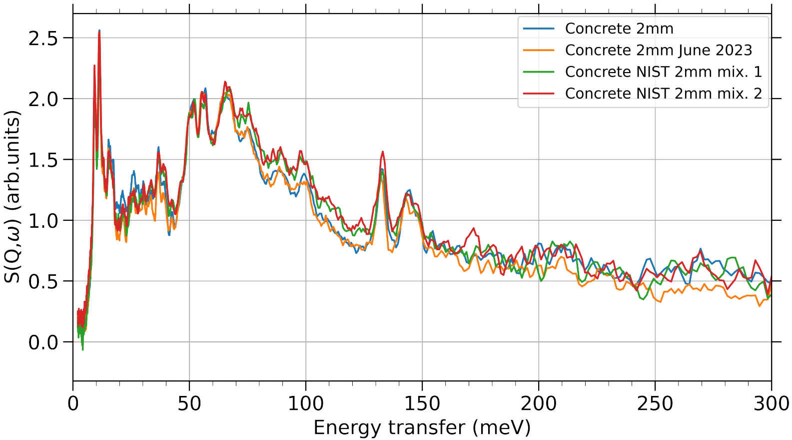
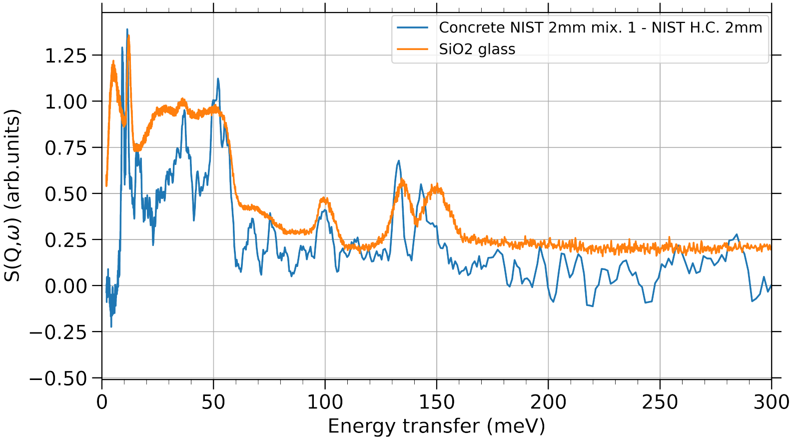
Concrete INS measurements



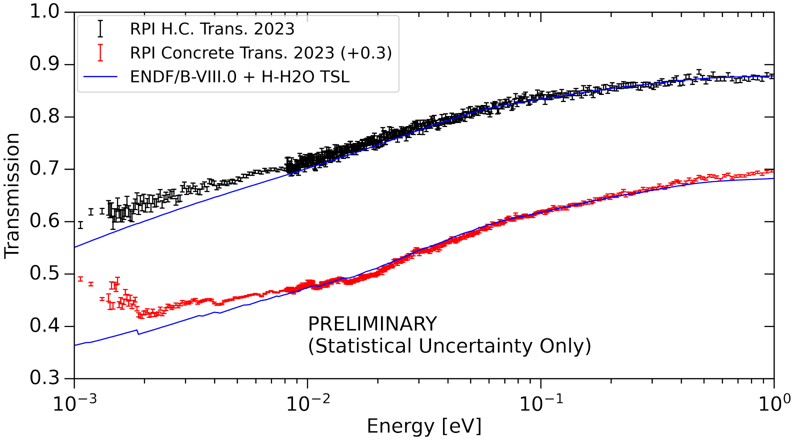
- Overall consistent shape of the measured $S(\alpha, \beta)$ spectra.

Concrete - H.C. INS comparison



- Albeit not the right thing to do considering sample thicknesses and content, the comparison with the quartz glass (which shows less crystallinity than quartz sand) confirms our hypothesis that the phonon spectra of concrete is a linear combination of H.C. and aggregates.

Concrete and H.C. transmission measurements



- Transmission measurement of concrete (due to appearance of Bragg edges) confirms our hypothesis that the transmission spectra of concrete is a linear combination of H.C. and aggregates.
- Accurate determination of water content is necessary.

Summary and future work

- INS measurements of different types of polyethylene have been carried out at ORNL.
- INS measurements of H.C. and concrete have been carried out at ORNL.
- Transmission measurements of H.C. and concrete at RPI.
- Linear combination hypothesis has been justified.
- Need to finish up atomistic modeling of hydrated cement.
- More INS and transmission measurements needed with different composition and aggregates.

Acknowledgements

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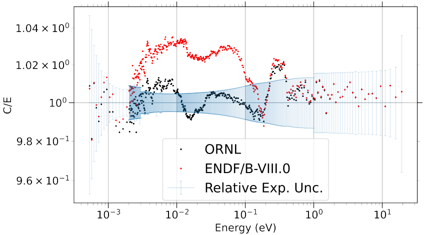
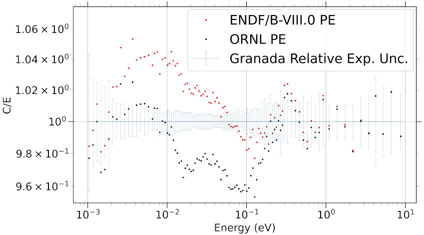
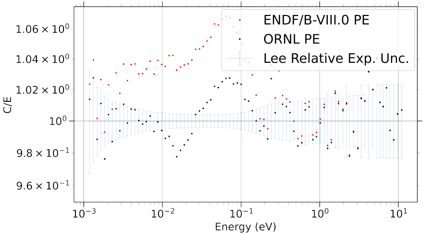
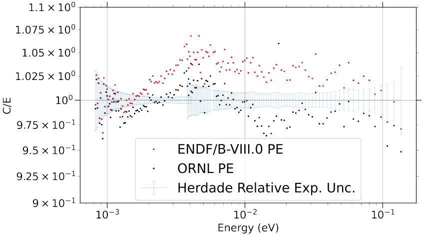
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

Additional slides: Polyethylene C/E other data









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