ORNL Neutron Imaging

NXS 2022

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ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

The Neutron Imaging Team

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Mary-Ellen Donnelly,
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SNS Group Leader

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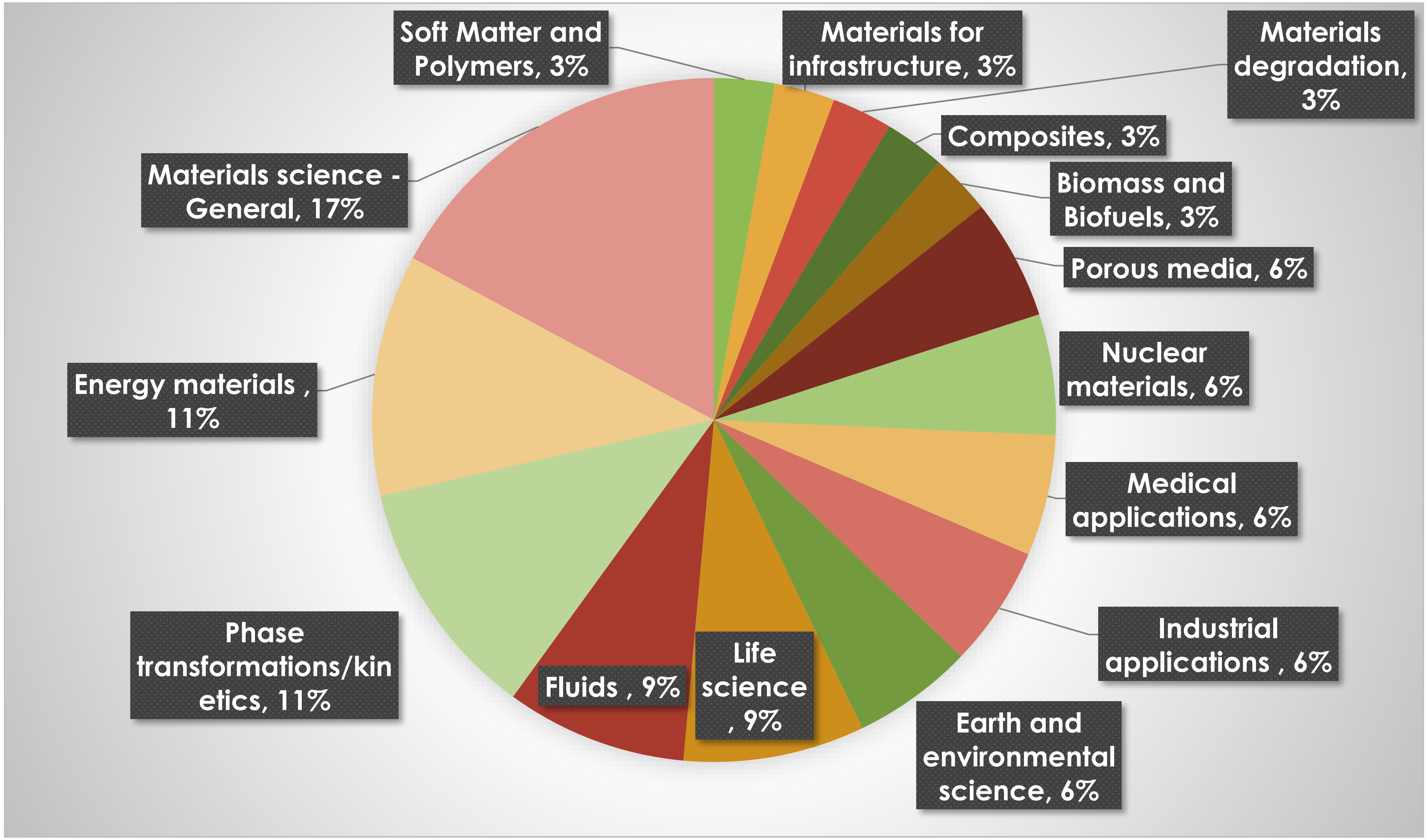
Imaging has a broad scientific portfolio



Imaging is a Growing Part of the ORNL Neutron Sciences Program

High Flux Isotope Reactor (HFIR)
Intense steady-state neutron flux
and a high-brightness cold neutron source

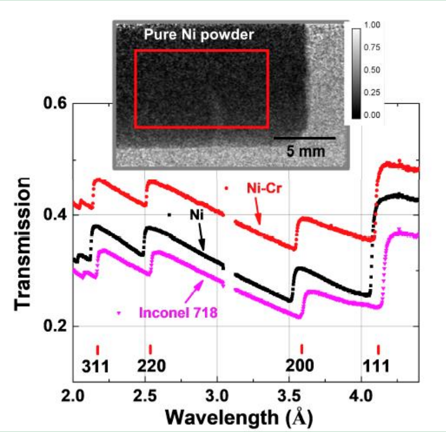
Dedicated Imaging Instrument (CG-1D)
Steadily improving capabilities
Expanded support

Spallation Neutron Source (SNS)
World's most powerful accelerator-based neutron source

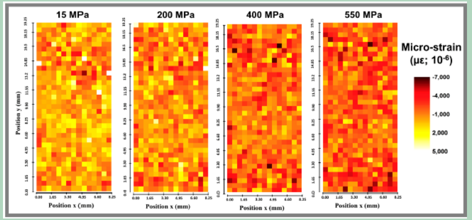
Techniques such as Bragg-edge imaging are being implemented on BL3 SNAP diffractometer (VENUS is under construction)

Future CUPI²D beamline at STS (Bragg edge and grating interferometry)

Bragg edge

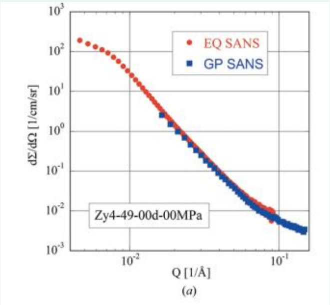


Transmission spectra of pure Ni, $Ni_{39}Cr_{11}$, and Inconel 718 powders.

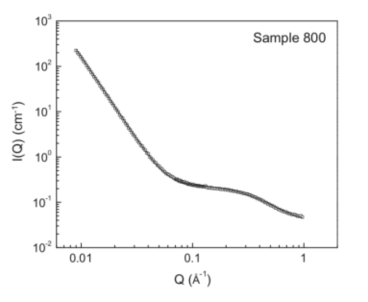


<200> Bragg edge strain map of additively manufactured Inconel 718 at 15, 200, 400 and 550 Mpa.

Scattering

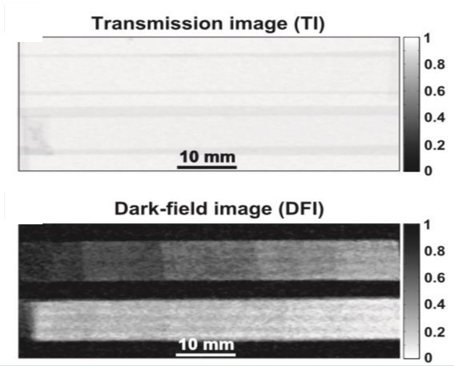


Radial average absolute differential macroscopic cross section vs. wavevector transfer in Zircaloy-4 cladding material

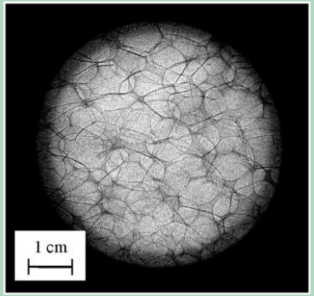


SANS raw data of microporous titanium carbide-derived carbon (TiC-CDC) at 800 C

Grating Interferometry

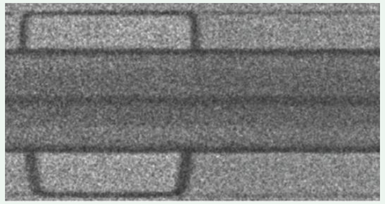


Radiograph (top) and Dark field image (bottom) of 1-10 μm layers of steel foil

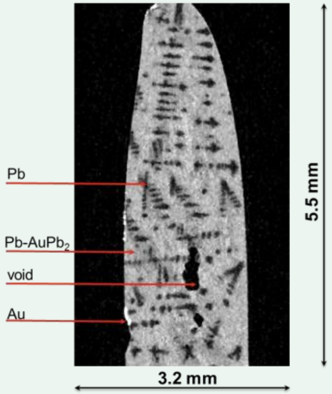


4 cm x 4 cm x 1 cm thick Al foam (invisible unless measured with gratings)

Microscopy

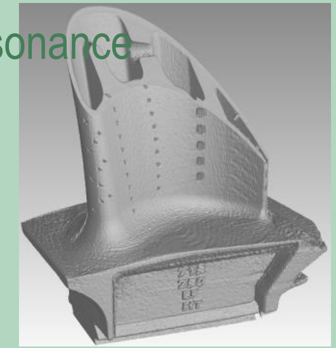


Radiograph of a membrane in a proton exchange membrane fuel cell (PEMFC) at a resolution of 1.98 μm

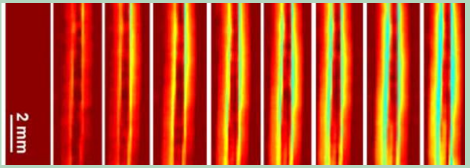


Vertical slice from a neutron microtomography dataset showing dendritic microstructures of lead, voids and gold in a sample of a gold-lead alloy

Radiography, Computed Tomography and Resonance



Cut through computed tomogram showing internal flow channels in an additively manufactured Inconel 718 turbine blade



Transmission radiographs at different stages of lithiation during the discharge process. Yellow and green colors indicate an increase in Li ion content in each cathode

Inferred structure (indirect)

Direct structure

0.1Å | 1.0nm | ← 0.1μm | 1.0 μm | 10.0μm | 10 cm

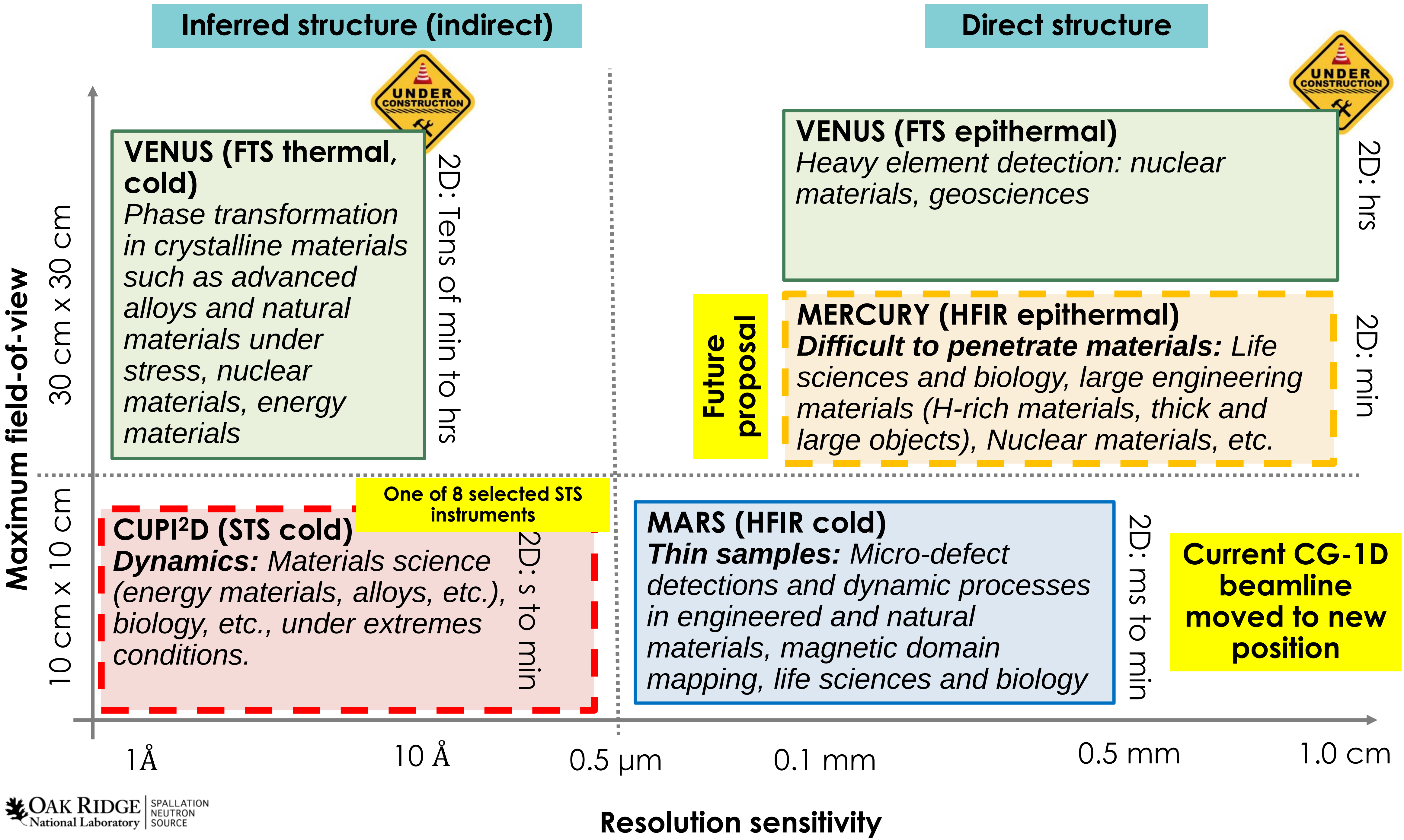
HFIR CG-1D/MARS (microscopy)

FTS VENUS (Bragg edge)

FUTURE PROPOSAL HFIR MERCURY (high penetration/large samples)

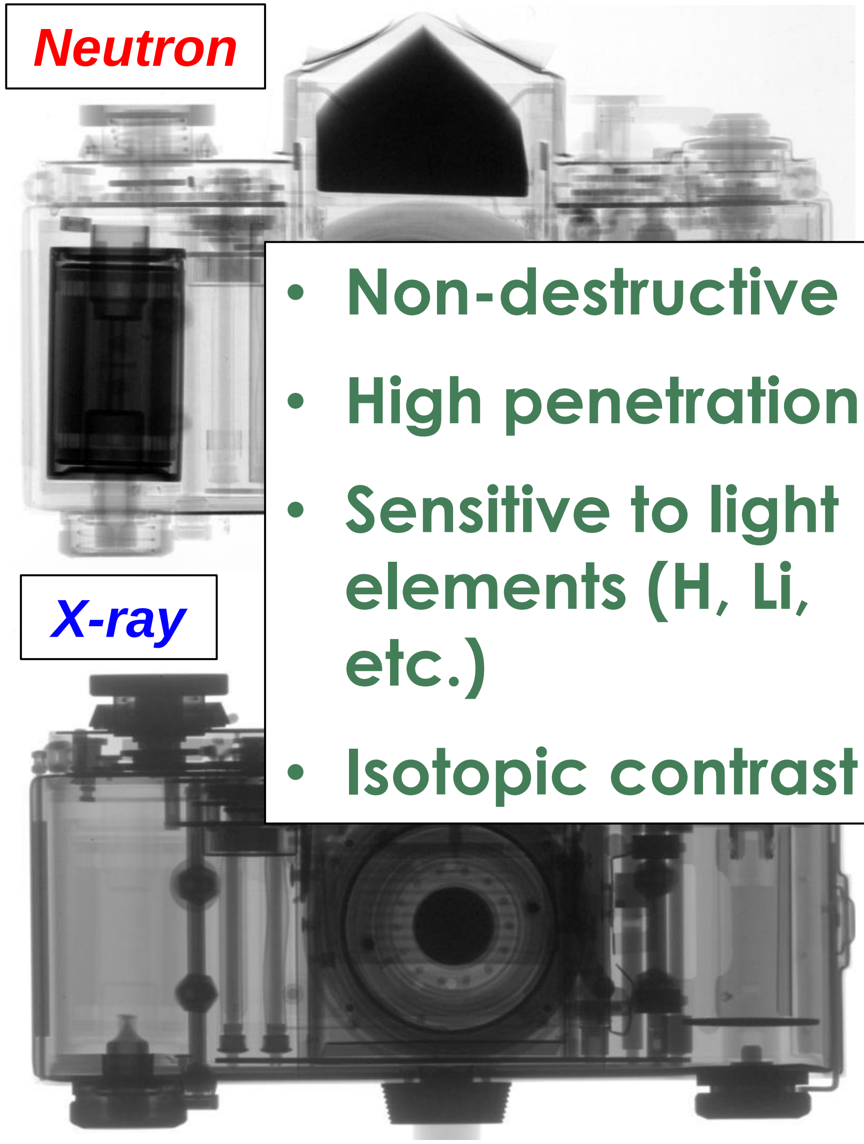
STS CUPI²D (combined Bragg edge and neutron grating interferometry)

STS VENUS (Resonance)



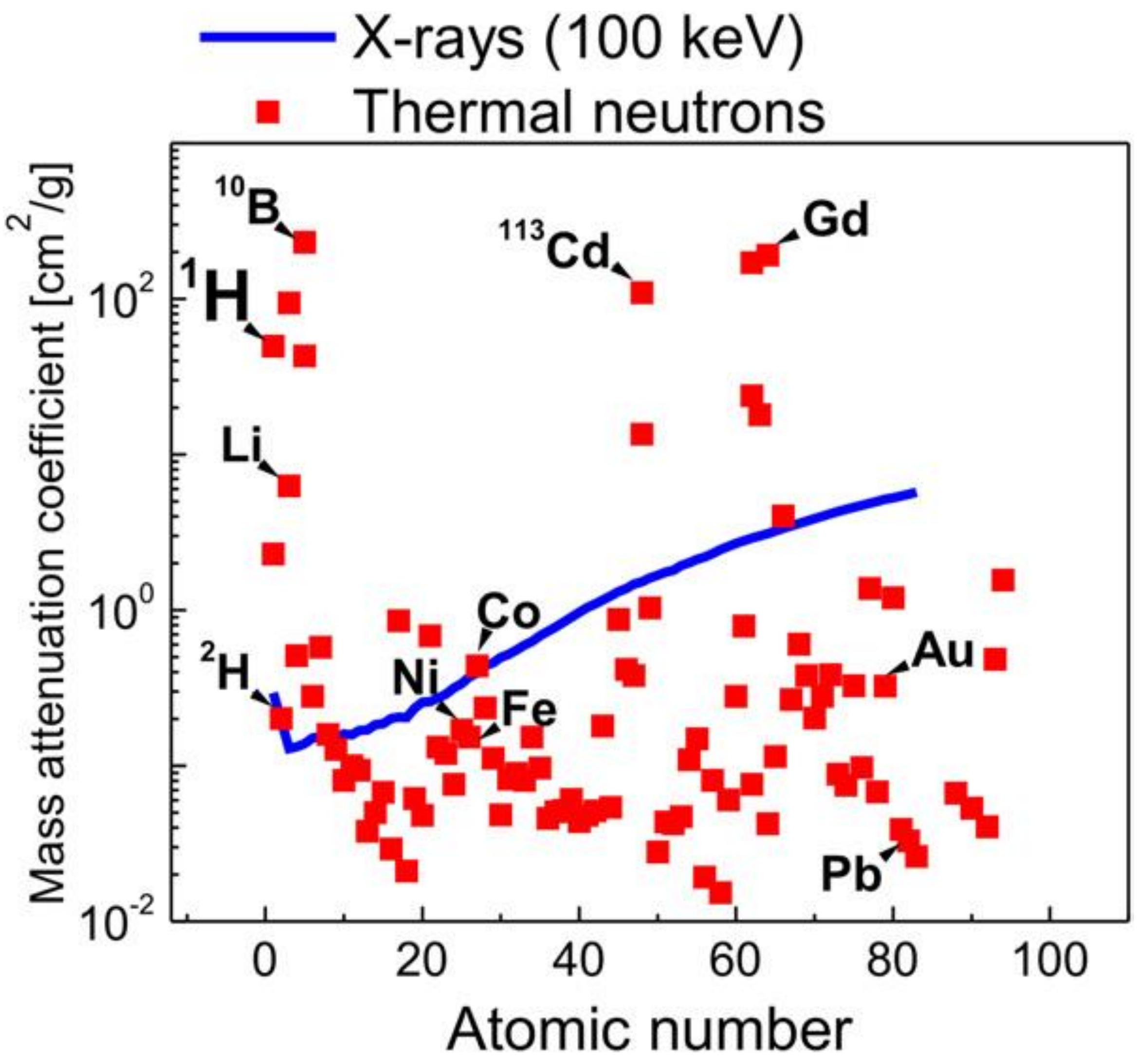
Inferred structure (indirect)
Direct structure
UNDER CONSTRUCTION
VENUS (FTS thermal, cold)
Phase transformation in crystalline materials such as advanced alloys and natural materials under stress, nuclear materials, energy materials
2D: Tens of min to hrs
UNDER CONSTRUCTION
VENUS (FTS epithermal)
Heavy element detection: nuclear materials, geosciences
2D: hrs
Future proposal
MERCURY (HFIR epithermal)
Difficult to penetrate materials: Life sciences and biology, large engineering materials (H-rich materials, thick and large objects), Nuclear materials, etc.
2D: min
One of 8 selected STS instruments
CUPI²D (STS cold)
Dynamics: Materials science (energy materials, alloys, etc.), biology, etc., under extremes conditions.
2D: s to min
MARS (HFIR cold)
Thin samples: Micro-defect detections and dynamic processes in engineered and natural materials, magnetic domain mapping, life sciences and biology
2D: ms to min
Current CG-1D beamline moved to new position
Maximum field-of-view
30 cm x 30 cm
10 cm x 10 cm
1Å
10 Å
0.5 µm
0.1 mm
0.5 mm
1.0 cm
Resolution sensitivity

Neutrons interact uniquely with matter



- Non-destructive
- High penetration
- Sensitive to light elements (H, Li, etc.)
- Isotopic contrast

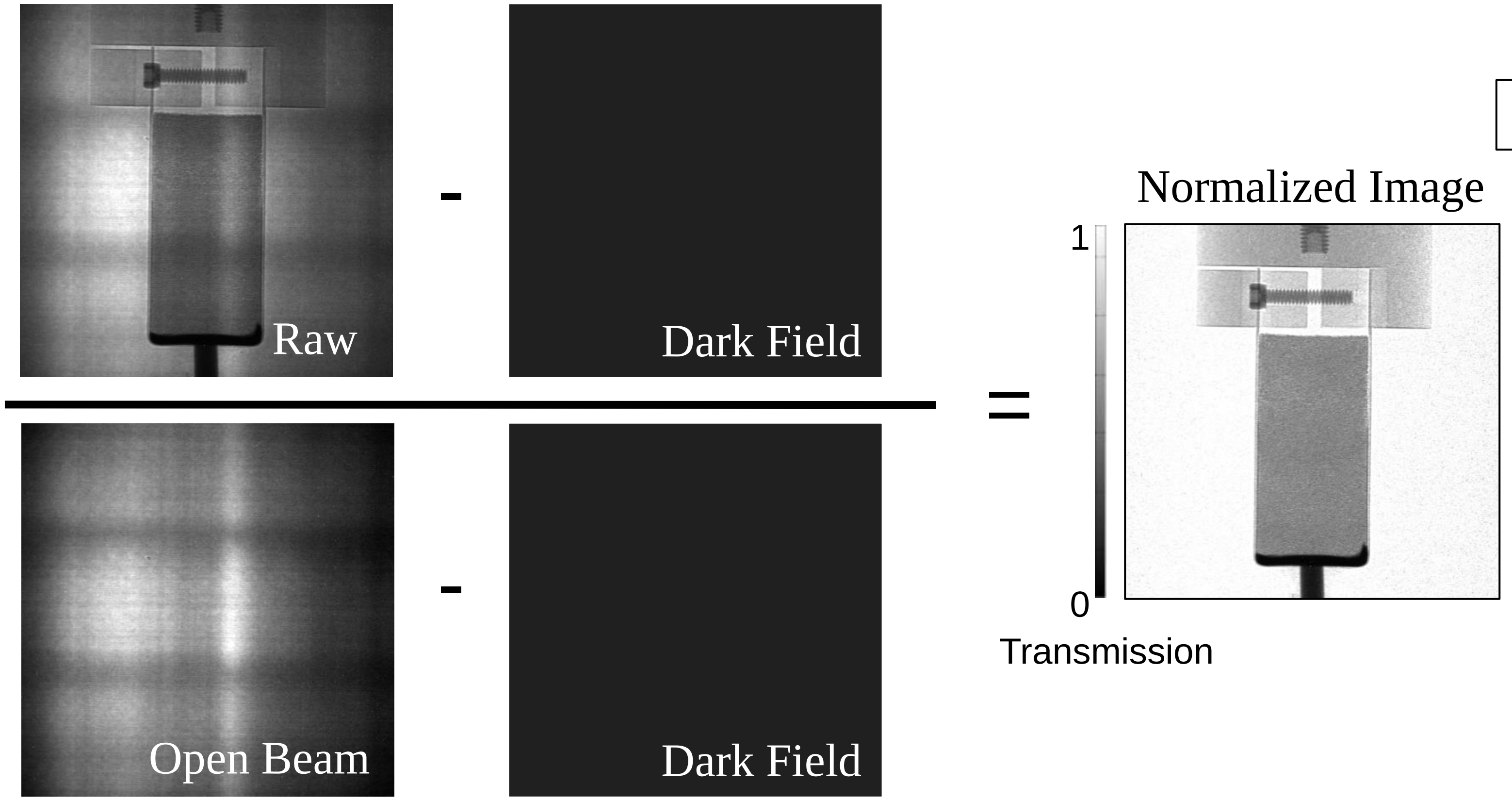
https://www.psi.ch/en/niag/what-is-neutron-imaging



[M. Strobl et al., J. Phys. D: Appl. Phys. **42** (2009) 243001]

OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

From raw image to normalized image



$$I_N(i,j) = \frac{I(i,j) - DF(i,j)}{OB(i,j) - DF(i,j)}$$

Lambert-Beer Law

$$T = \frac{I}{I_0} = e^{-\mu x}$$

Transmission (T), Sample thickness (x), Attenuation co. (μ)

$$\mu = \sigma_{tot} \frac{\rho N_A}{M}$$

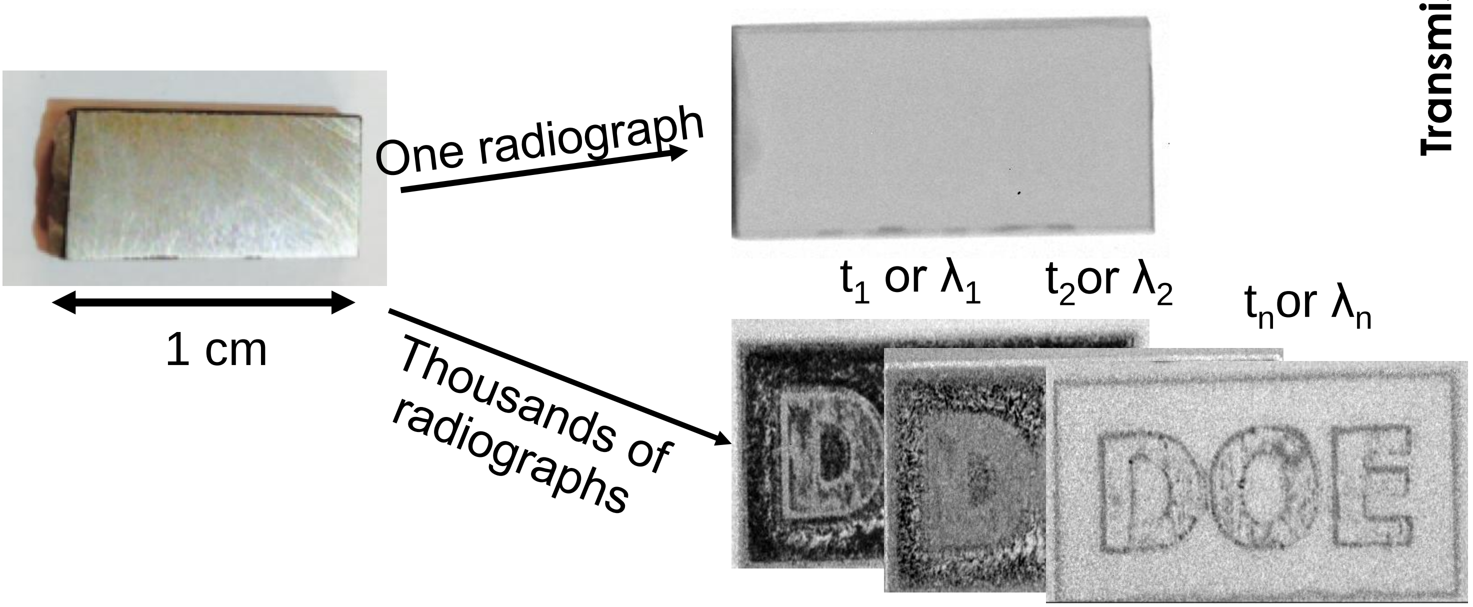
Density (ρ), Avogadro constant (N_A), Total cross-section (σ_{tot}), Molar mass (M)

Principle of Bragg edge imaging (using cold neutrons)

- Spallation neutron sources discriminate neutron wavelength (or energy) by using the time-of-flight (TOF) technique

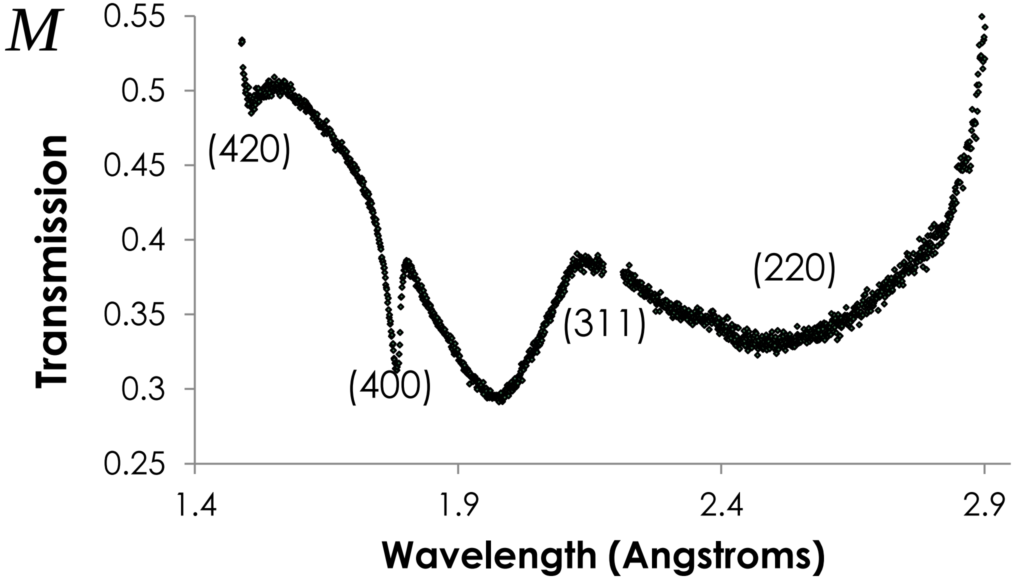
$$I(\lambda) = I_0(\lambda)e^{-\mu(\lambda)x} \qquad \mu(\lambda) = \sigma_t(\lambda)\frac{\rho N_A}{M}$$

White-beam (or reactor-based) neutron radiograph:
sums over all neutron wavelengths



Wavelength-dependent (or TOF) neutron radiographs (**Discrete** neutron wavelengths)

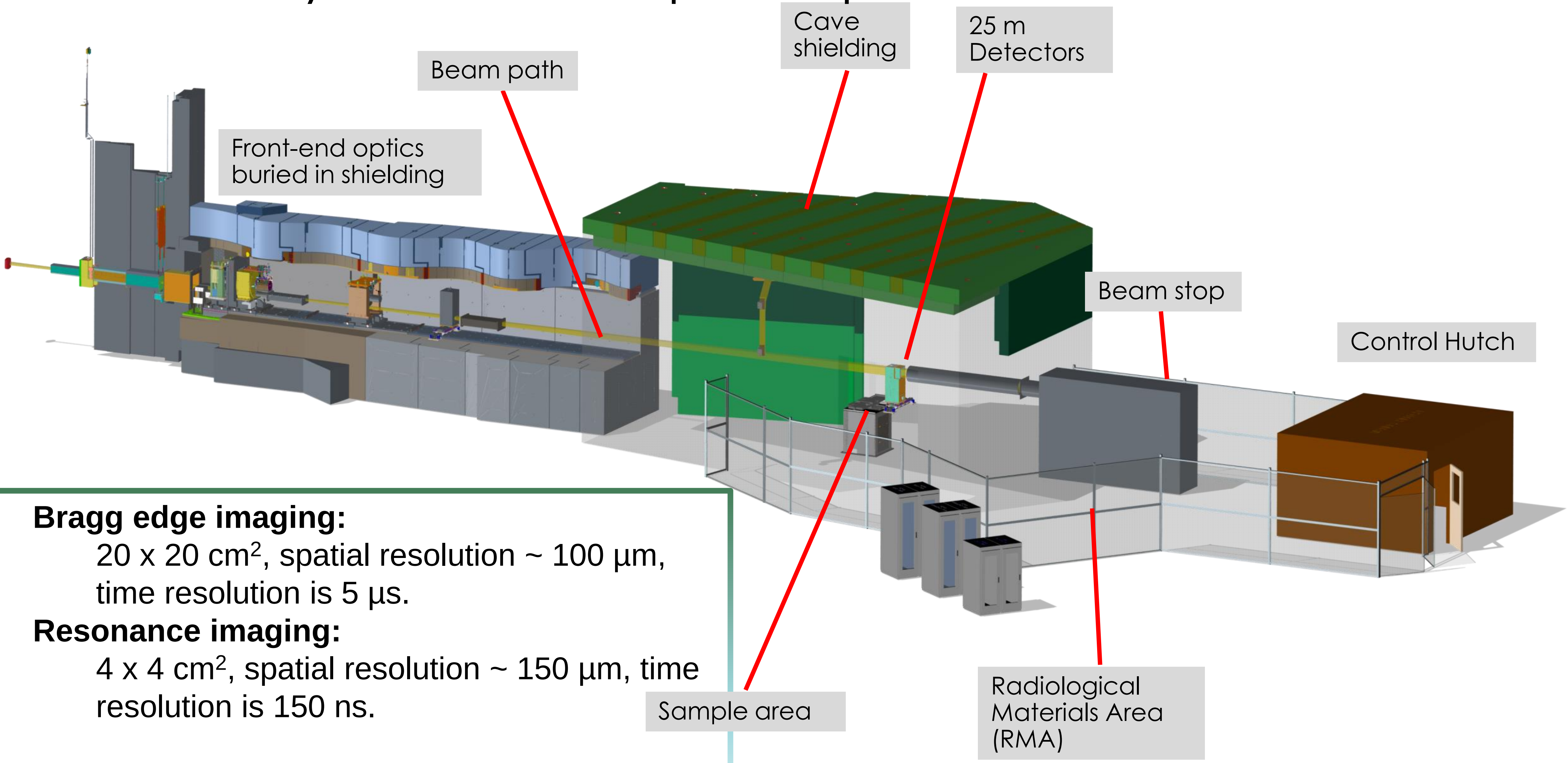
Wavelength range ~ [1-10 Å]



Position of the edge gives the d-spacing of <hkl> or displacement gives the strain

Barton J.P., Bilheux H.Z., Bossi R., Herwig K.W., Santodonato L., Taylor M., "Chapter 12: Neutron Radiography for Nondestructive Testing", *Nondestructive Testing Handbook, Fourth Edition: Volume 3, Radiographic Testing (RT)* (2019).

VENUS layout and unique capabilities



Bragg edge imaging:

20 x 20 cm^2, spatial resolution ~ 100 µm, time resolution is 5 µs.

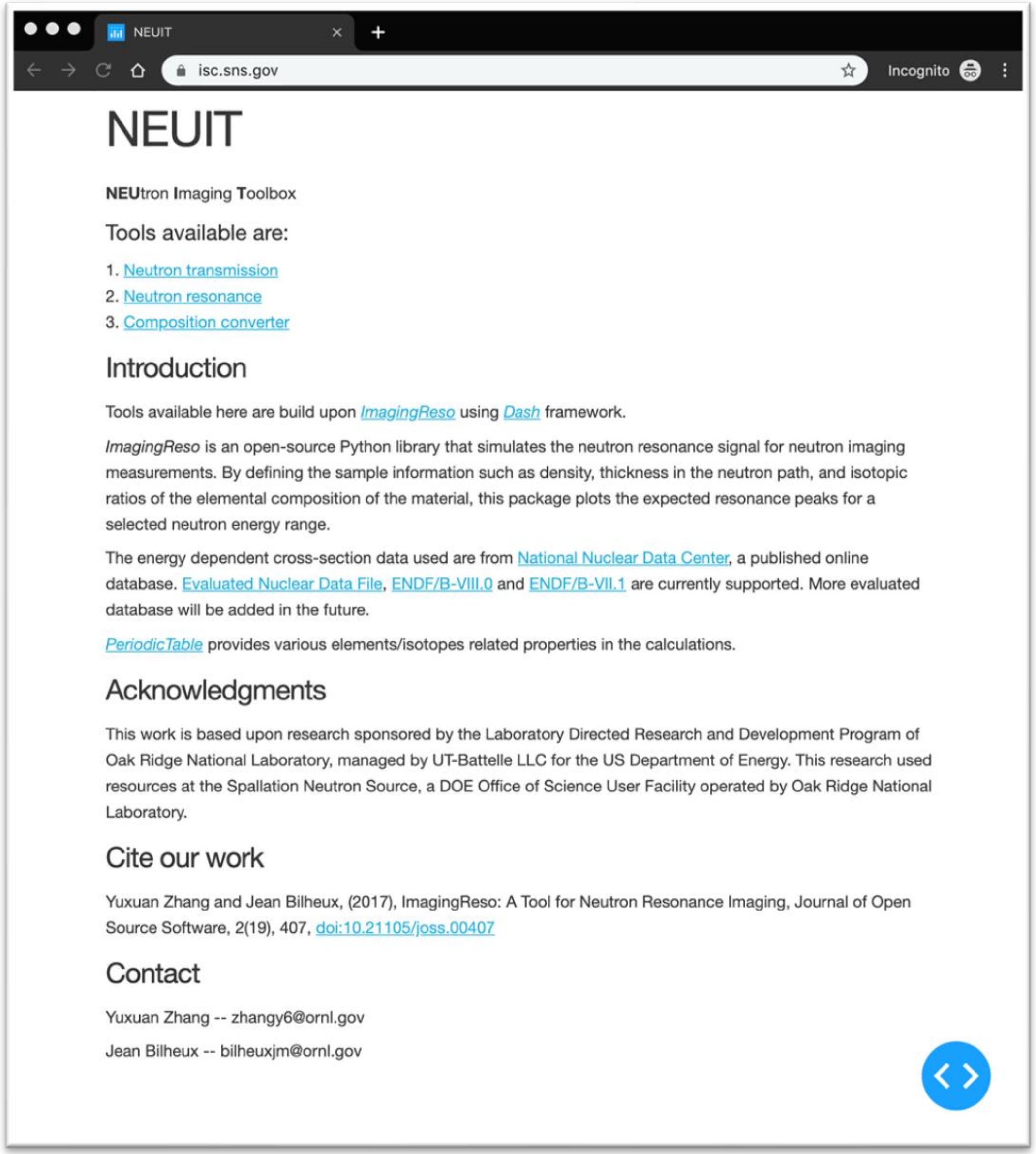
Resonance imaging:

4 x 4 cm^2, spatial resolution ~ 150 µm, time resolution is 150 ns.

Preparing for an imaging experiment

- Predict overall transmission in your sample (iNEUIT)
- Contact instrument team to optimize your experimental measurements (detector, SNR, sample environment, etc.)
- Contact computational instrument scientist to discuss data processing and analysis requirements (Python Jupyter notebooks)

Experiment planning tools: *NEUIT* (**NEU**tron **I**maging **T**oolbox)



NEUIT

isc.sns.gov

NEUIT

NEUtron **I**maging **T**oolbox

Tools available are:

1. Neutron transmission
2. Neutron resonance
3. Composition converter

Introduction

Tools available here are build upon *ImagingReso* using *Dash* framework.

ImagingReso is an open-source Python library that simulates the neutron resonance signal for neutron imaging measurements. By defining the sample information such as density, thickness in the neutron path, and isotopic ratios of the elemental composition of the material, this package plots the expected resonance peaks for a selected neutron energy range.

The energy dependent cross-section data used are from National Nuclear Data Center, a published online database. Evaluated Nuclear Data File, ENDF/B-VIII.0 and ENDF/B-VII.1 are currently supported. More evaluated database will be added in the future.

PeriodicTable provides various elements/isotopes related properties in the calculations.

Acknowledgments

This work is based upon research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle LLC for the US Department of Energy. This research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by Oak Ridge National Laboratory.

Cite our work

Yuxuan Zhang and Jean Bilheux, (2017), ImagingReso: A Tool for Neutron Resonance Imaging, Journal of Open Source Software, 2(19), 407, doi:10.21105/joss.00407

Contact

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- Tools available:
  1) Neutron transmission
     Compute white-beam transmission
  2) Neutron Resonance
     Simulate energy-dependent signal
  3) Composition convertor
     Perform wt. % <==> at. % conversion
- Nuclear database supported
  - ENDF/B-VIII.0 (BNL)
  - ENDF/B-VII.1 (BNL)
- Elemental/isotopic info
  - PeriodicTable 1.5.0 (NIST)

NEUtron **I**maging **T**oolbox (*NEUIT*, https://neuit.sns.gov/)

For white-beam imaging at CG-1D

Home

Neutron resonance

Cold neutron transmission

Sample info

+ -

Chemical formula	Thickness (mm)	Density (g/cm³)
H2O	2	1
Al		

NOTE: density input can be omitted (leave as blank) only if the input formula is single element, density available here will be used.

☐ Modify isotopic ratios

SUBMIT

(demo)

Result

Transmission:

The total neutron transmission at CG-1D (ORNL): 50.902 %

Attenuation:

The total neutron attenuation at CG-1D (ORNL): 49.098 %

Sample stack:

Layer 1: H2O

Thickness (mm)	Density (g/cm³)
2	1

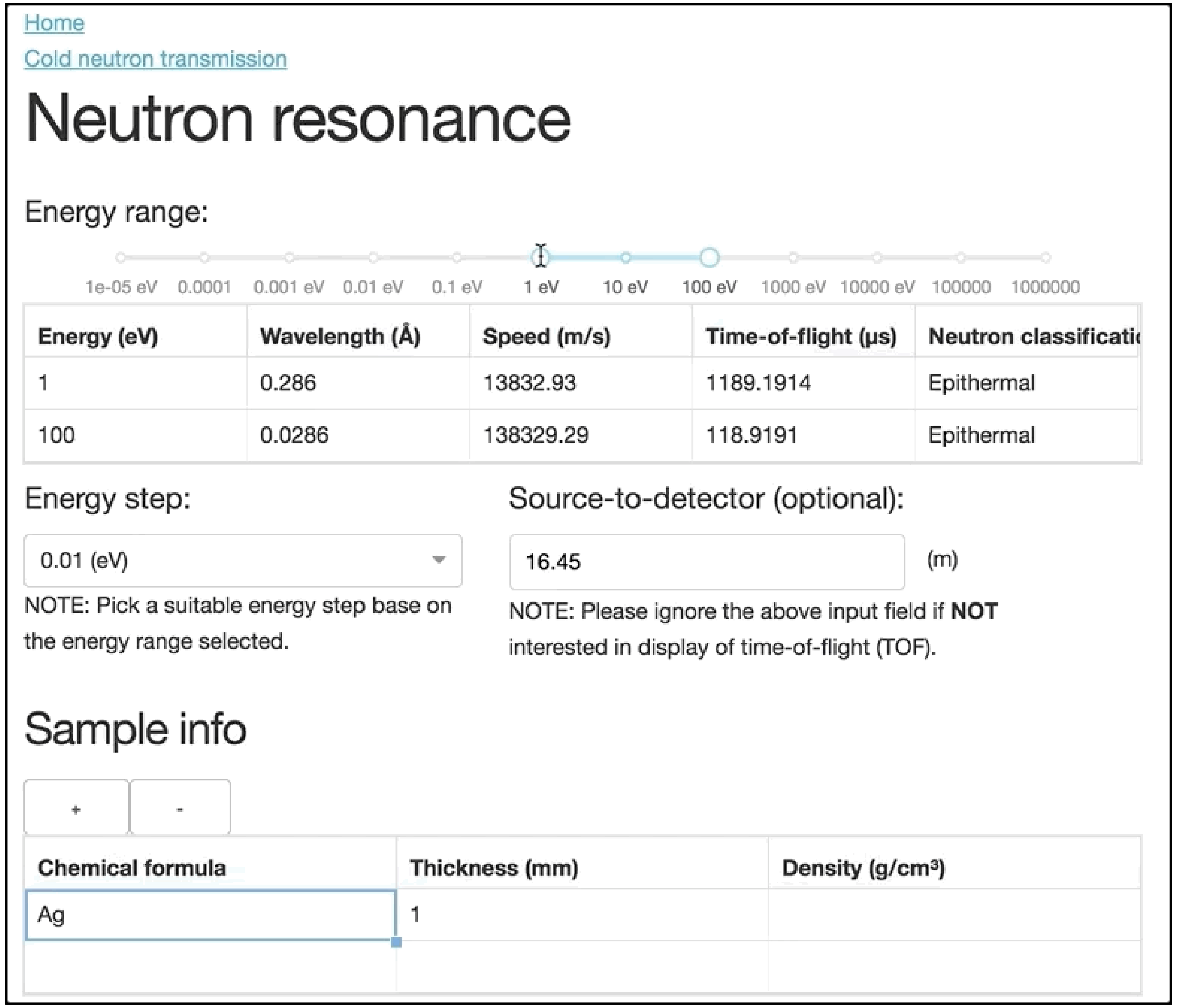
1-H	2-H	3-H
0.9999	0.0001	0

16-O	17-O
0.9976	0.0004

(static)

NEUtron **I**maging **T**oolbox (*NEUIT*, https://neuit.sns.gov/)

For resonance imaging



(demo)

(static)

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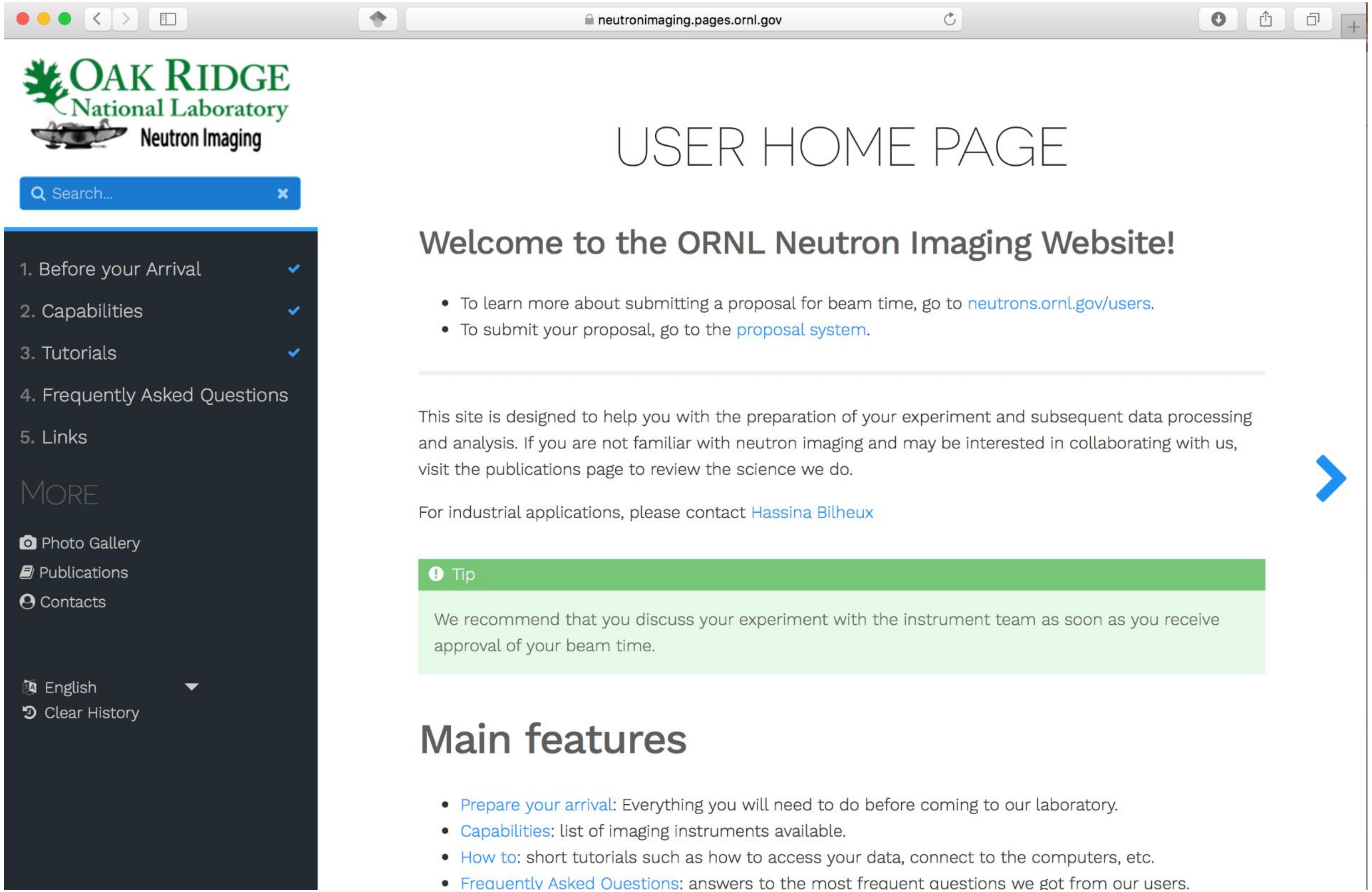
Jupyter Notebooks Demonstration

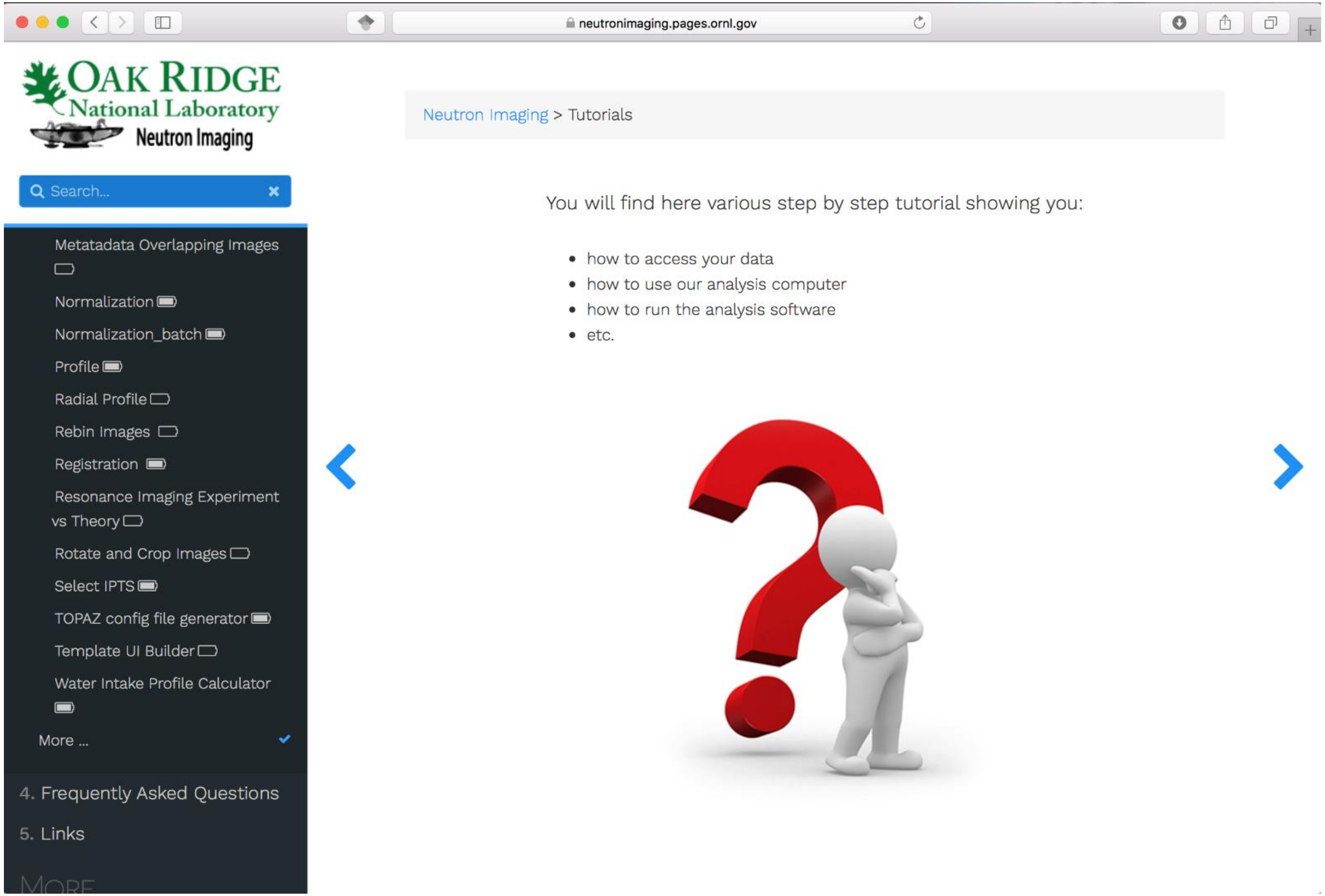
- Samples: Ni and Cu powders in Al cans measured at SNS BL-03 SNAP
- Goals:
  - Load and normalized data in iBeatles software
  - Plot and Identify Bragg edges
  - Fit Bragg edges
  - Calculate d-spacing

How to get to analysis server and start iBeatles

- On a web browser, type “analysis.sns.gov”
- Enter username and password
- On analysis server, open a terminal window
- Type: /SNS/users/j35/bin/start/iBeatles

We have a user home page with instructions and tutorials





Step-by-step tutorials with animated demonstrations

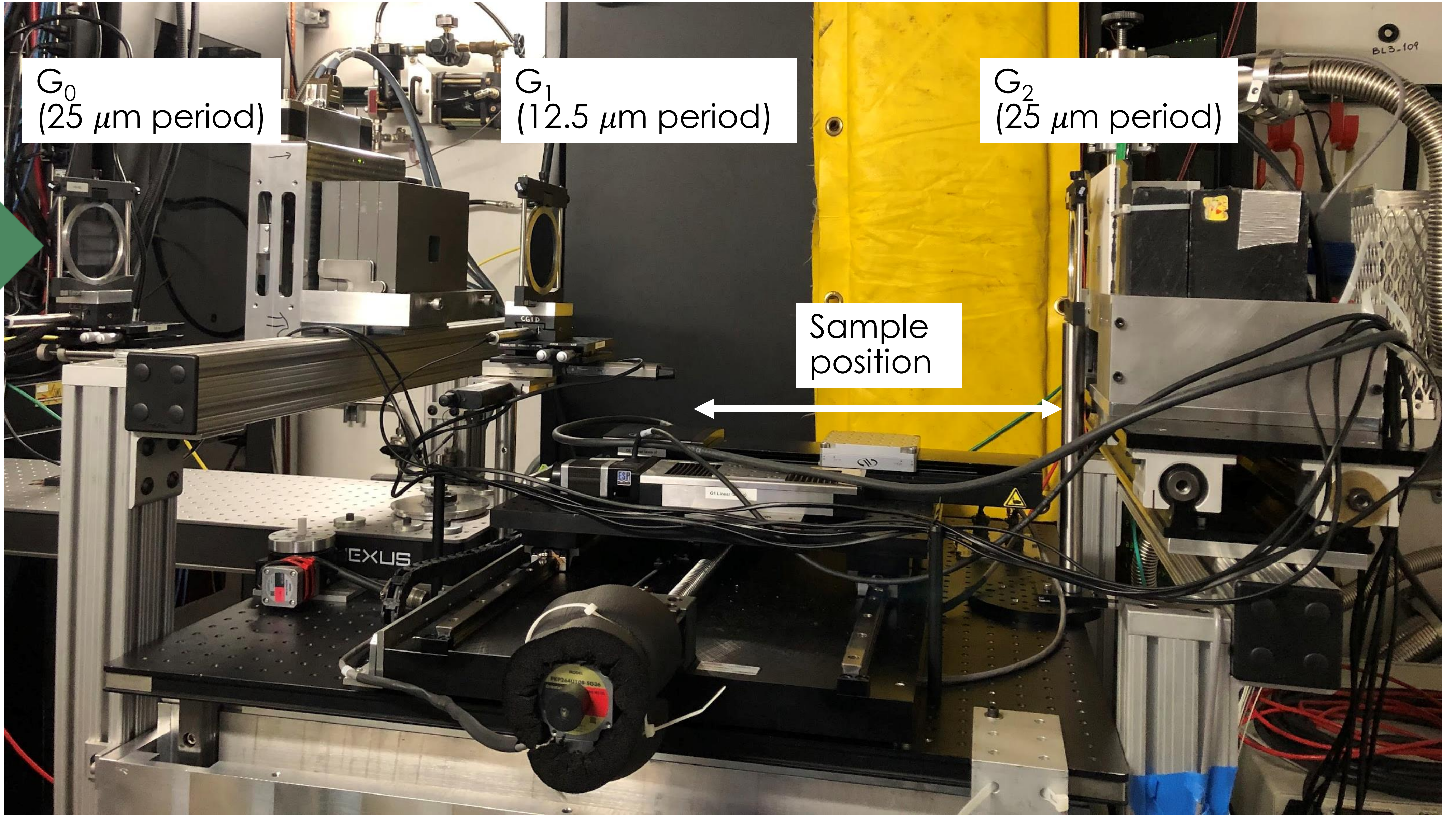
Something you want to see on our user website? Contact Jean Bilheux bilheuxjm@ornl.gov

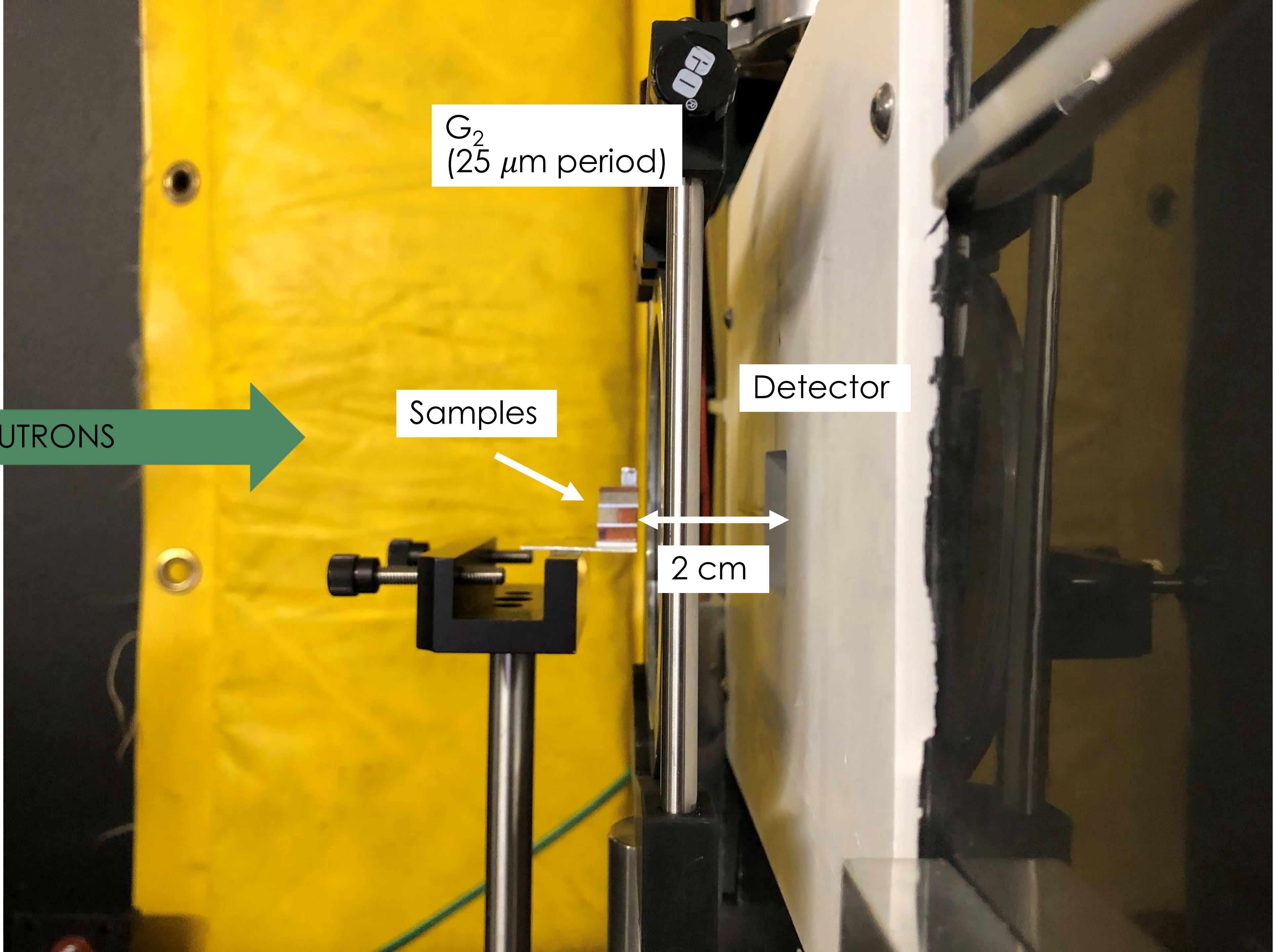
https://neutronimaging.pages.ornl.gov/

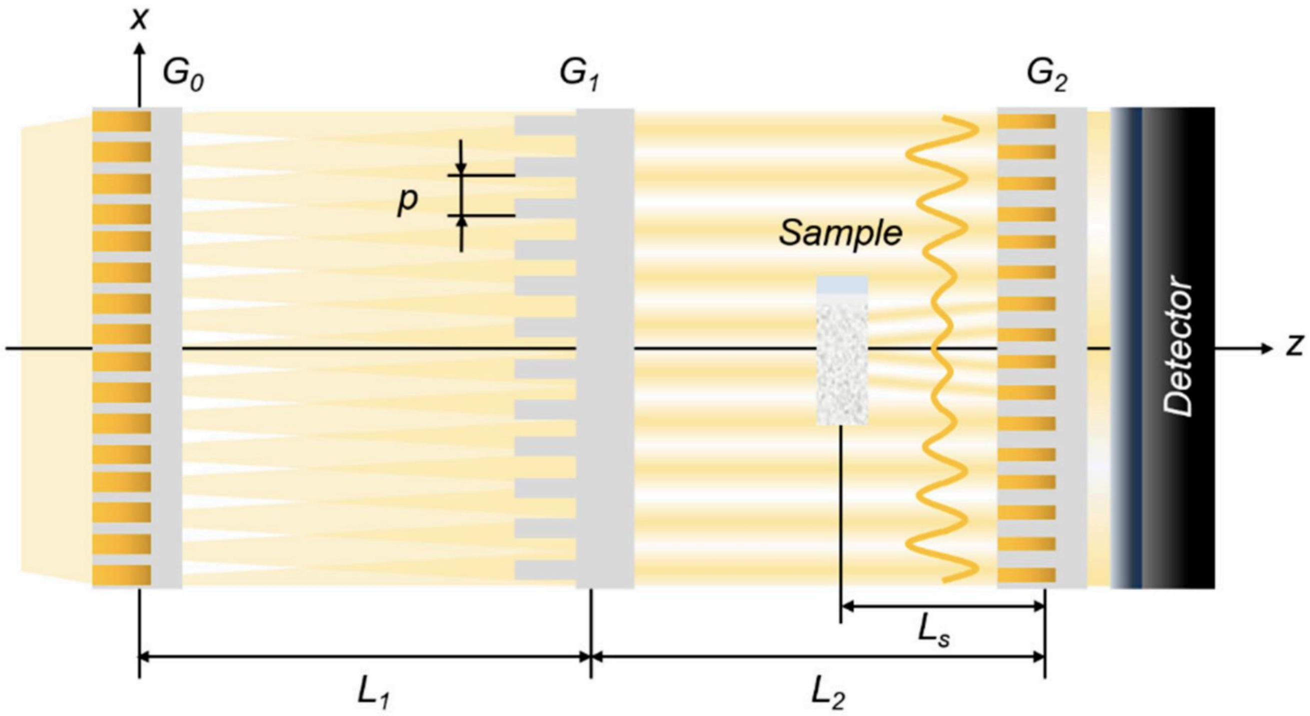
This week's imaging experiment: time-of-flight neutron grating interferometry

- International collaboration between:
  - Markus Strobl and Matteo Busi, Paul Scherrer Institute, Switzerland
  - Simon Sebold, TUM-FRM-II, Germany
  - ORNL neutron imaging team
- We are measuring the small angle scatter the sample produces when interacting with neutrons:
  - This is called the dark field imaging technique
  - We are using a symmetric grating system (i.e., equidistance between the 3 gratings) because it can accept a broad band of neutrons will keeping good visibility

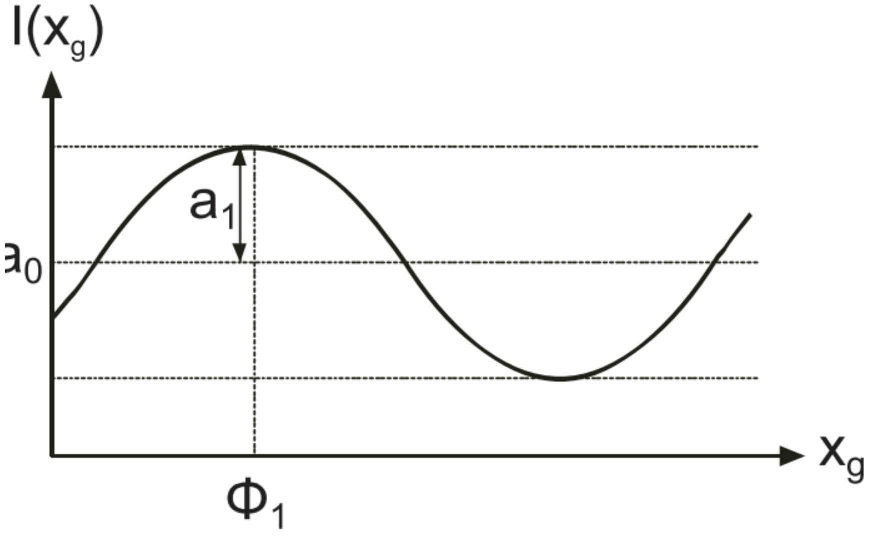
This week's imaging experiment: time-of-flight neutron grating interferometry




G_2
(25 μm period)
Detector
Samples
NEUTRONS
2 cm



Modulation pattern on every detector pixel obtained by stepping G1 perpendicular to beam



$$\xi = \lambda L_s / p$$

$$V = (I_{max} - I_{min})/(I_{max} + I_{min})$$

Grünzweig, C., Quantification of the neutron dark-field imaging signal in grating interferometry. Physical Review B - Condensed Matter and Materials Physics, 88(12), 1–6. https://doi.org/10.1103/PhysRevB.88.125104

Kim, Y.; Valsecchi, J.; Oh, O.; Kim, J.; Lee, S.W.; Boue, F.; Lutton, E.; Busi, M.; Garvey, C.; Strobl, M. Quantitative Neutron Dark-Field Imaging of Milk: A Feasibility Study. Appl. Sci. 2022, 12, 833. https:// doi.org/10.3390/app12020833

Example of DFI Data Analysis

Visibility is related to real-space correlation

$$V_s(\xi_{GI})\big/V_0(\xi_{GI}) = e^{\int_{path}\Sigma(G(\xi_{GI})-1)dt}$$

For dilute solution of spherical particles

Cross section

Volume fraction

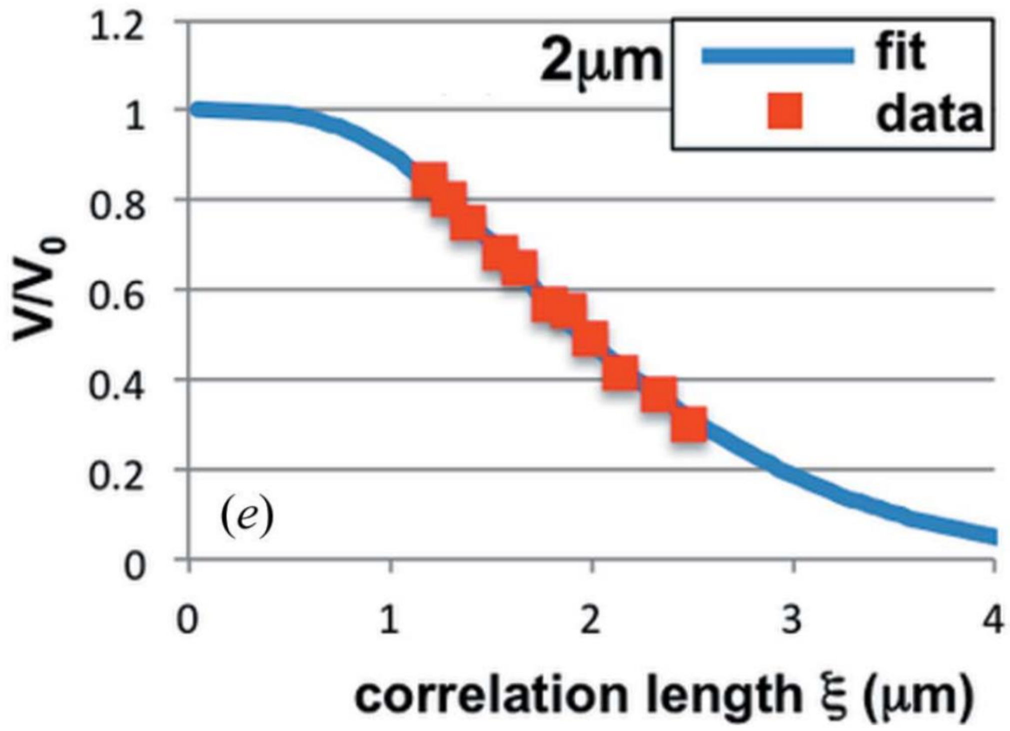
Scattering length density contrast

Radius

$$\Sigma_s = (3/2)\varphi_V \Delta\rho^2\lambda^2 r$$

Correlation length

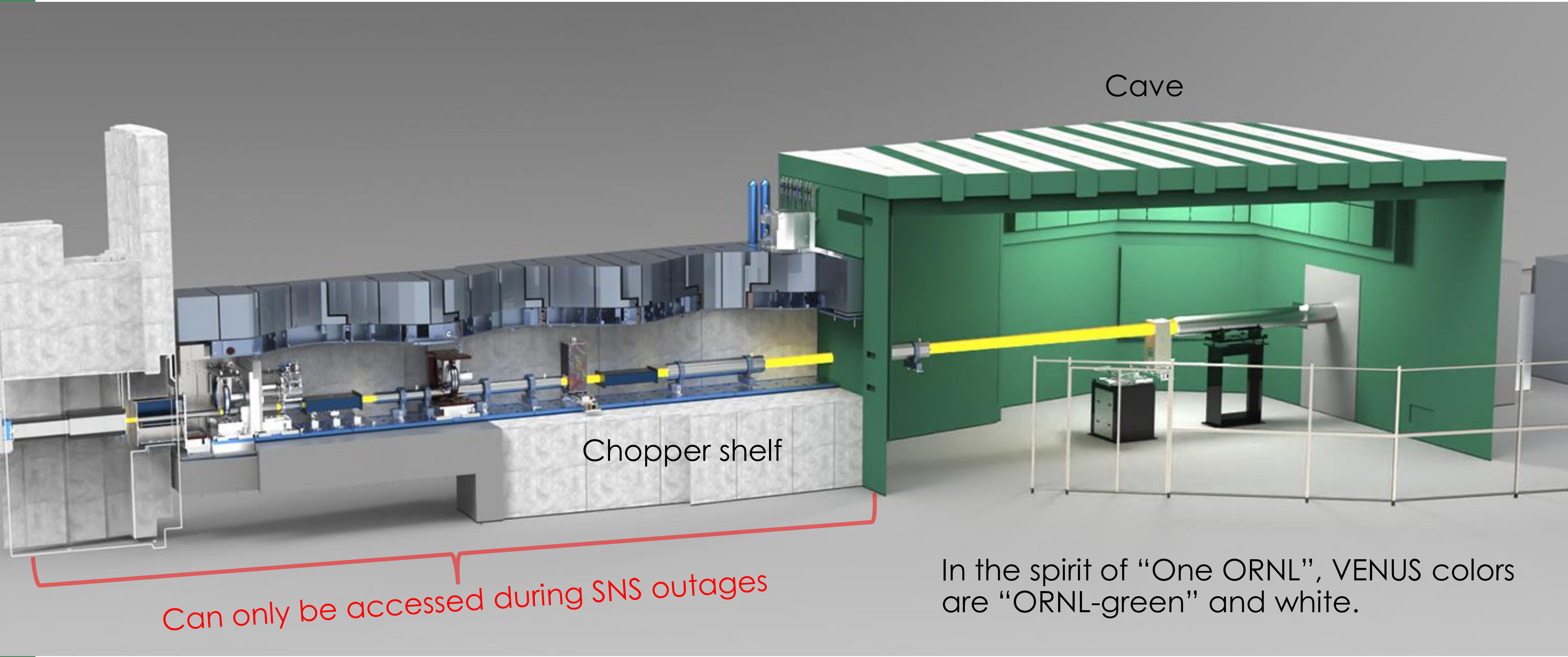
$$G(\zeta) = G(\xi/r) = \left[1-\left(\frac{\zeta}{2}\right)^2\right]^{1/2}\left(1+\frac{1}{8}\zeta^2\right) + \frac{1}{2}\zeta^2\left[1-\left(\frac{\zeta}{4}\right)^2\right] ln\left[\frac{\zeta}{2+(4-\zeta^2)^{1/2}}\right]$$



Strobl, M. (2015) 'General solution for quantitative dark-field contrast imaging with grating interferometers', *Scientific Reports*, 4(1), p. 7243. Available at: https://doi.org/10.1038/srep07243.

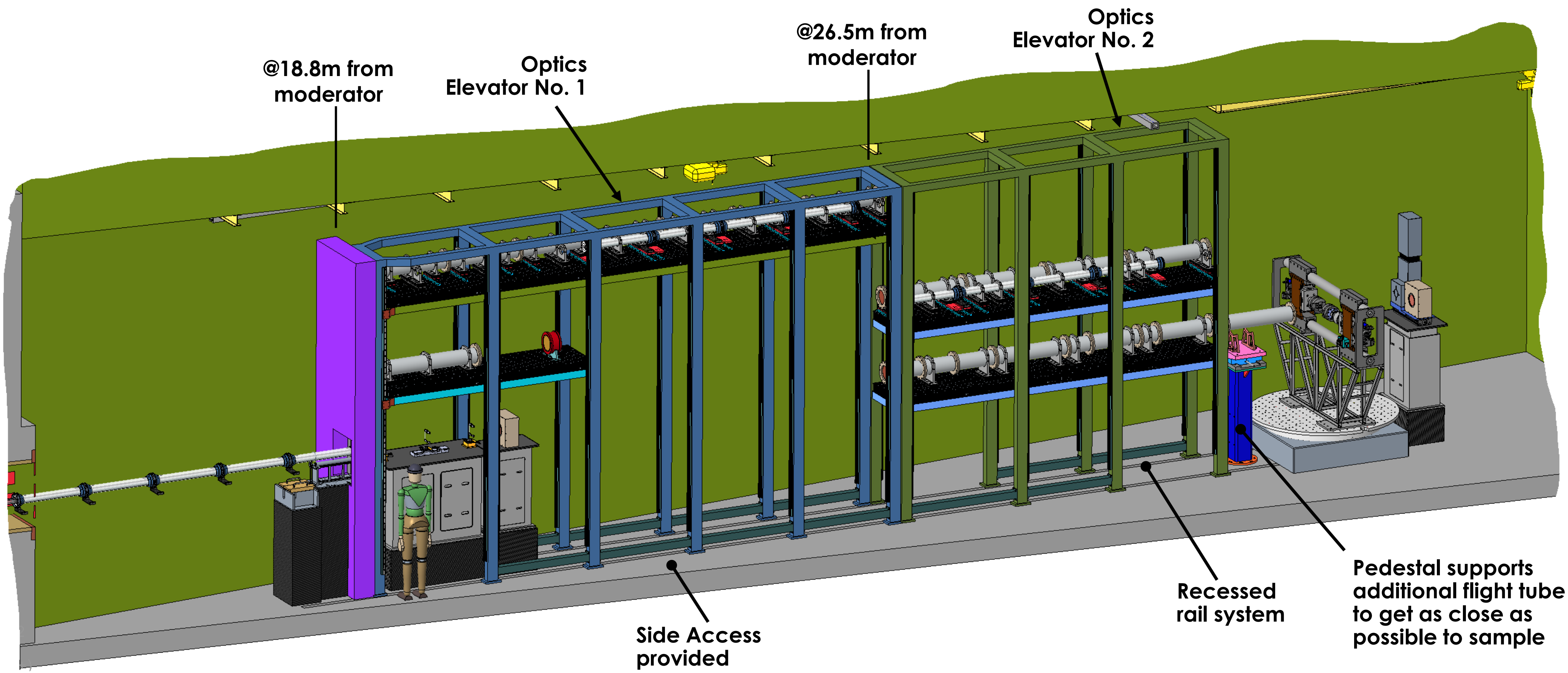
Strobl, M. *et al.* (2016) 'Wavelength-dispersive dark-field contrast: micrometre structure resolution in neutron imaging with gratings', *Journal of Applied Crystallography*, 49(2), pp. 569–573. Available at: https://doi.org/10.1107/S1600576716002922.

Artistic rendering of VENUS



In the spirit of “One ORNL”, VENUS colors are “ORNL-green” and white.

CUPI²D's Current Conceptual Design




CG-1D
NEUTRON IMAGING BEAMLINE
NEUTRON SCATTERING
INSTRUMENT