VENUS on the horizon: time-of-flight imaging capabilities for Earth and planetary materials

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3rd In-situ Studies of Rock Deformation NSF Research Coordination Network

The Hotel at the University of Maryland

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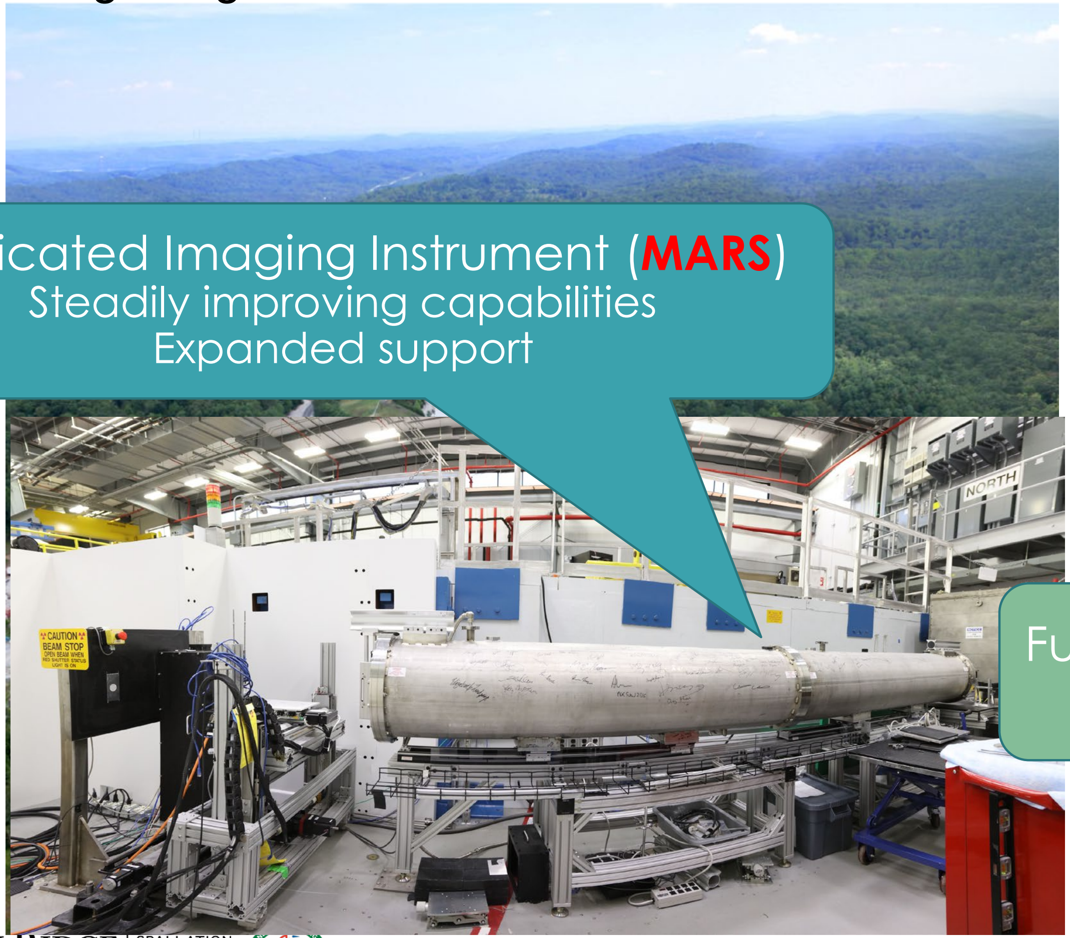
Outline

- **Neutron imaging at ORNL**
- Principle of time-of-flight (TOF) or hyperspectral neutron imaging
- Resonance imaging
- Bragg edge imaging
- Software efforts
- VENUS
- Conclusion

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

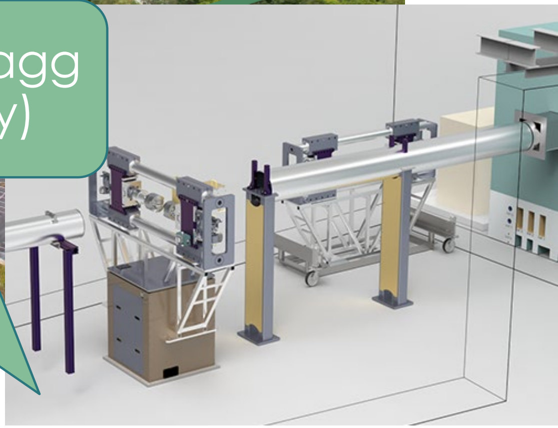


Dedicated Imaging Instrument (**MARS**)
Steadily improving capabilities
Expanded support

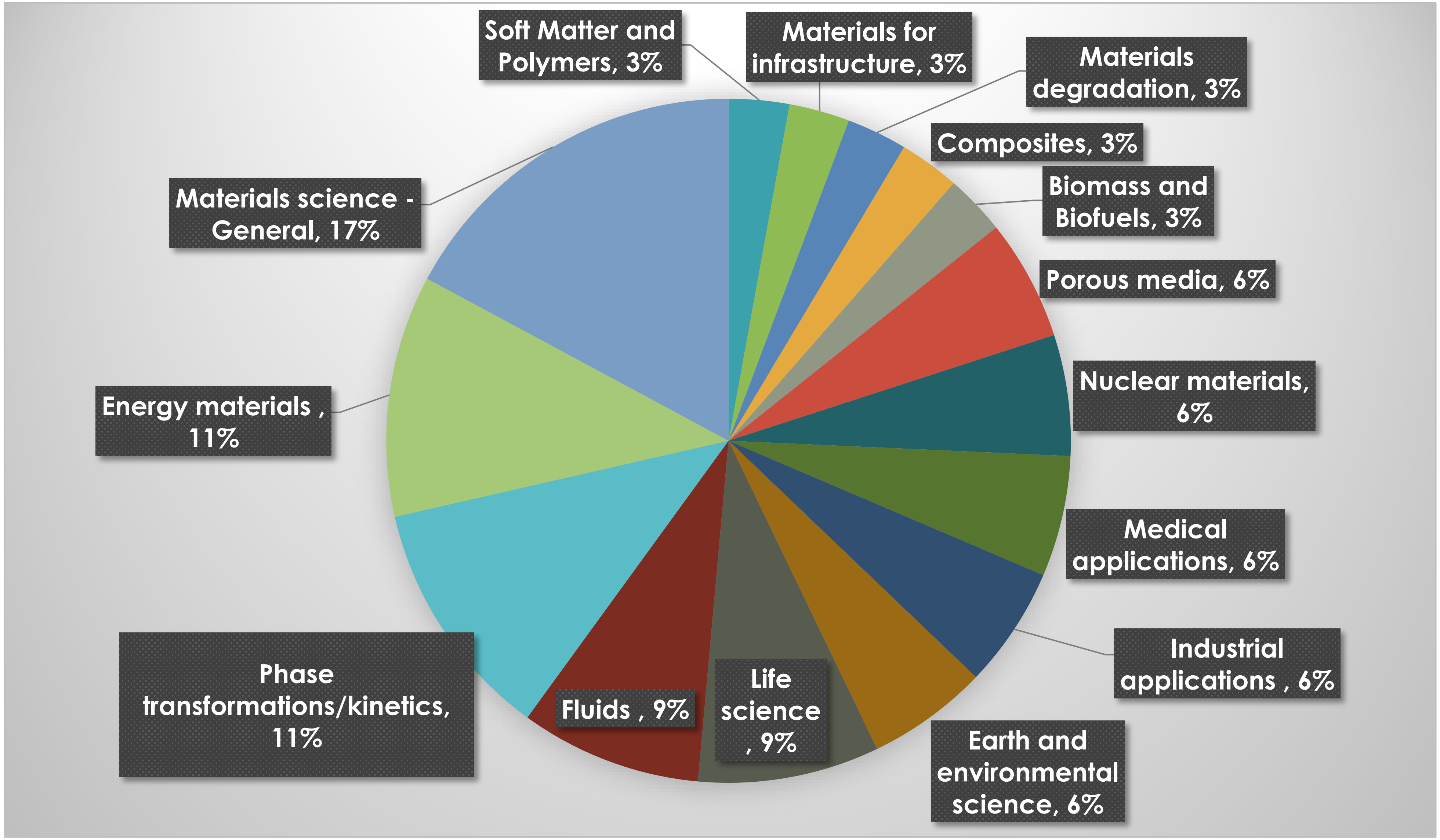
Spallation Neutron Source (SNS)
World's most powerful accelerator-based neutron source

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

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



Neutron imaging has a *broad* scientific portfolio



- ✓ Studies "real world" systems
- ✓ Structural measurements
- ✓ Real-time *in situ* functioning of systems
- ✓ Software essential to successful experiment
- ✓ Advances in Machine Learning

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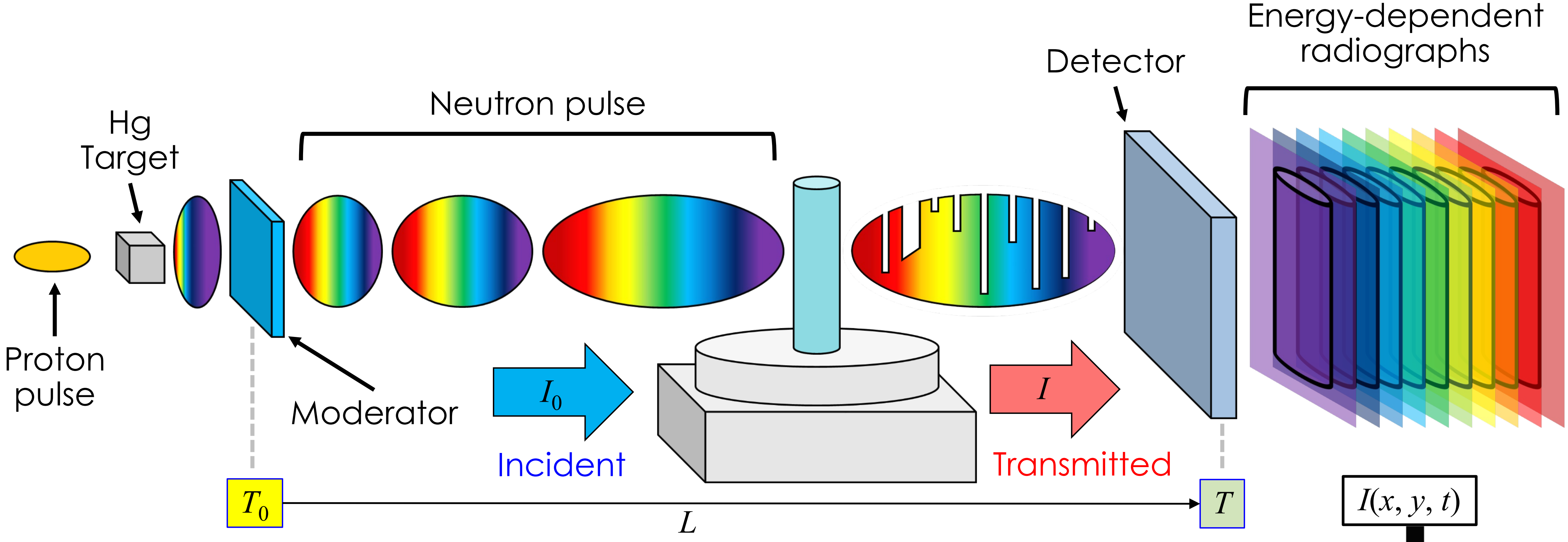
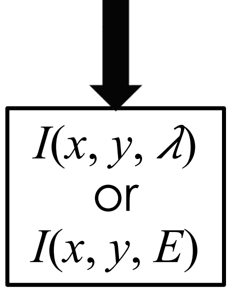
The Spallation Neutron Source layout

Imaging at a pulsed source (SNS)



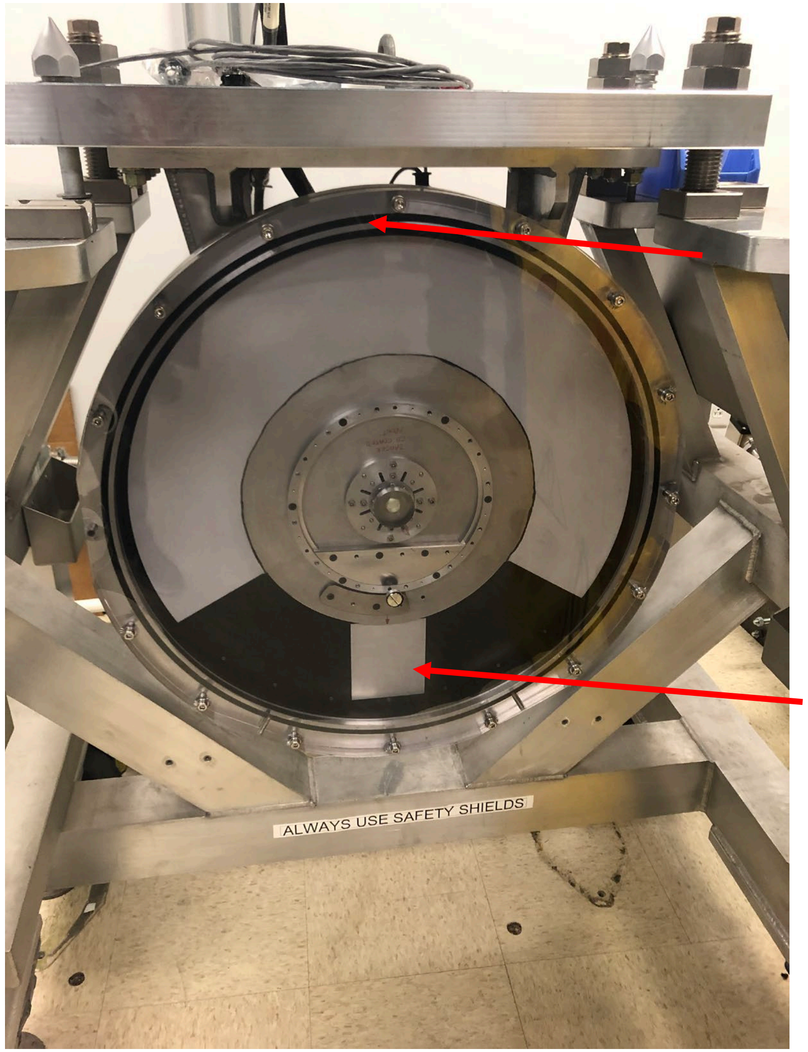
Courtesy of Y. Zhang, ORNL



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

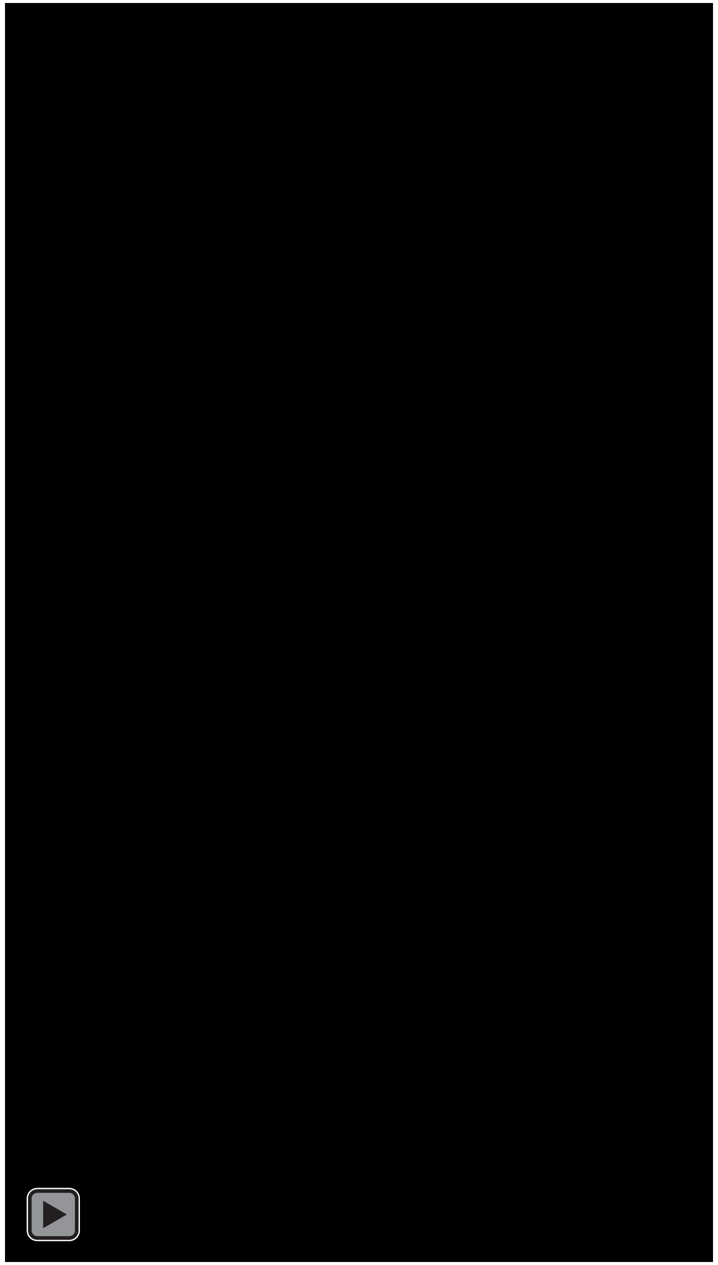
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

Disk chopper



1.0 mm of $^{10}B_4C$ and 1.6 mm of epoxy to get 1x 10^{-5} transmission at 1 Å

Disk chopper neutron window



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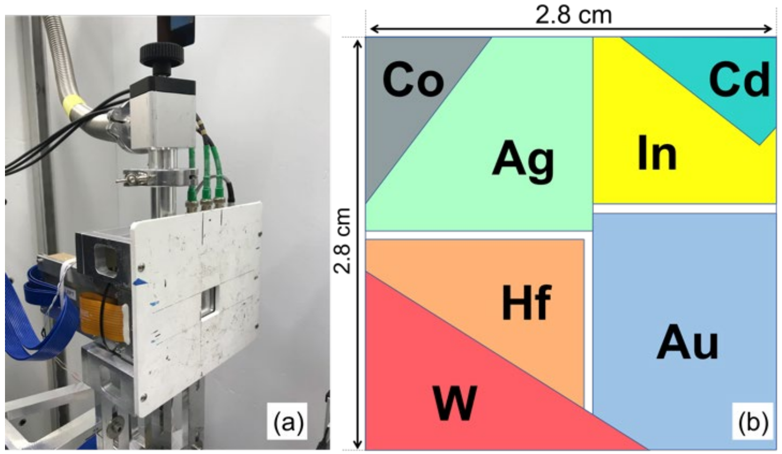
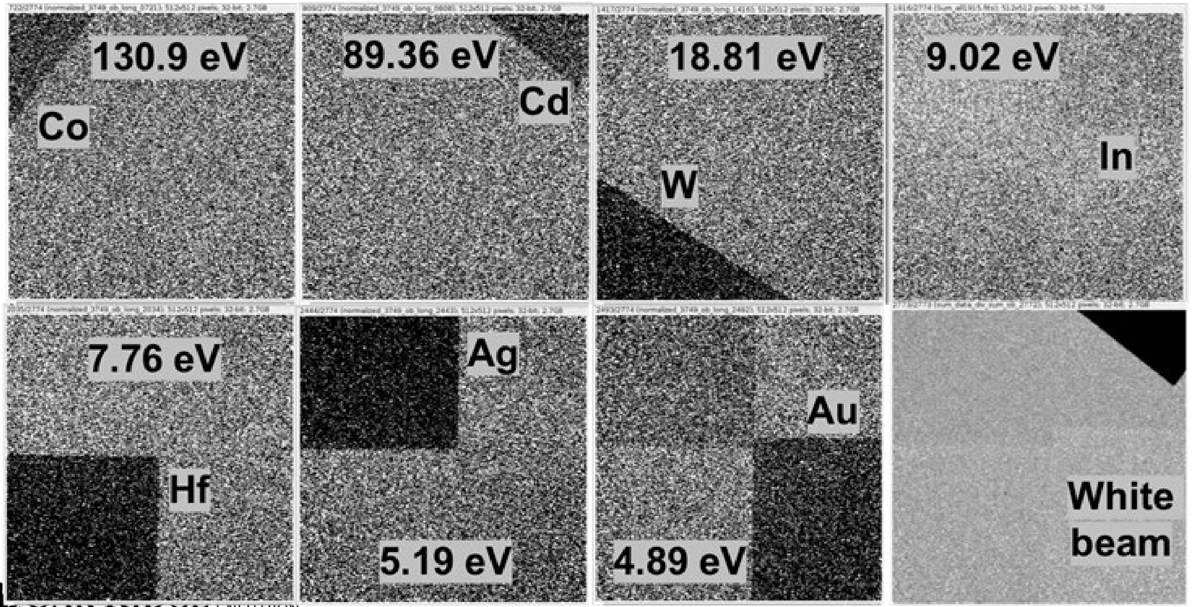
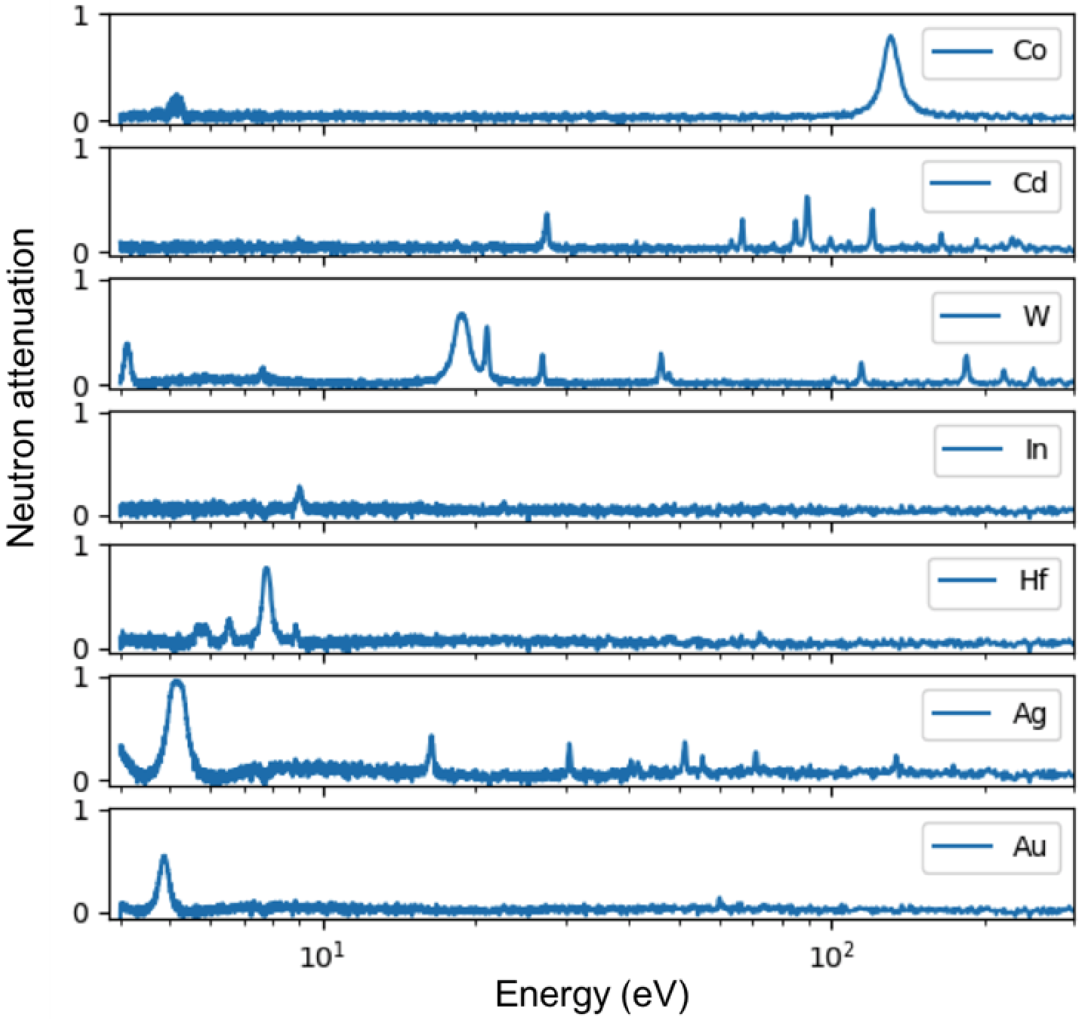
Higher energy neutrons can also be used for imaging (neutrons of energies higher than 1 eV): Resonance Imaging



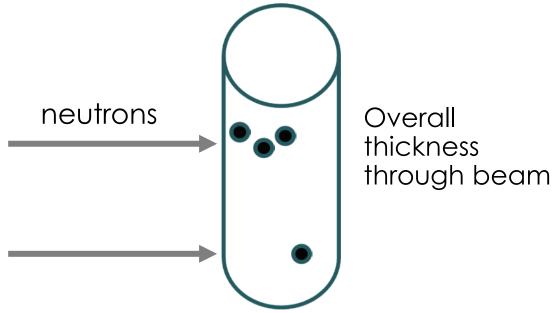




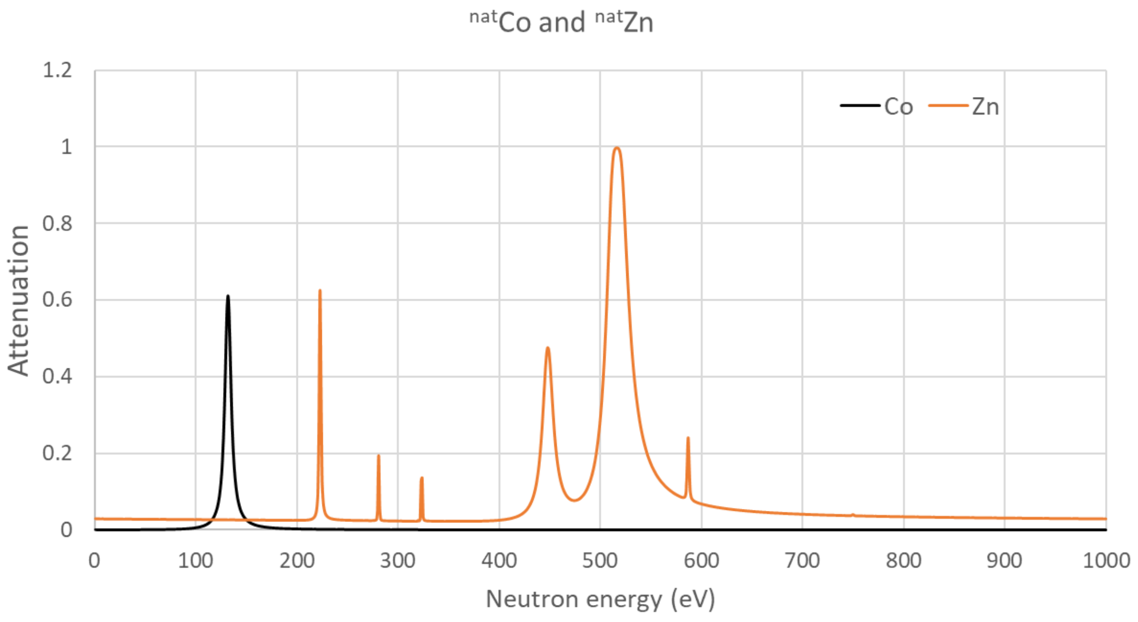
Zhang Y., Myhre K.G., Bilheux H.Z., Tremsin A.S., Johnson J.A., Bilheux J., Miskowiec A., Hunt R.D., Santodonato L., Molaison J.J., "Neutron Resonance Radiography and Application to Nuclear Fuel Materials", *Transactions of the American Nuclear Society,* (2018).

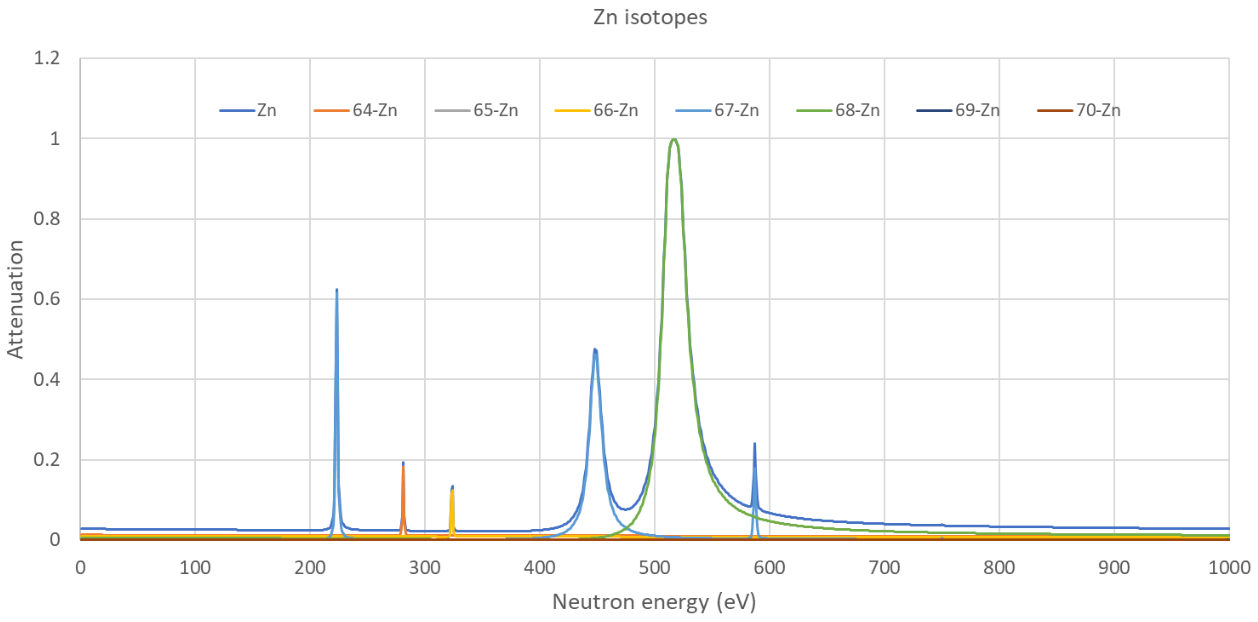
Scientific applications that benefit from resonance imaging

- Soil surveys, contaminants in soil, etc.:
  - transmission through 0.01 mm thickness of ^{nat}Co (between 1 and 5 Å) = 99.5 %
  - transmission through 1 mm thickness of ^{nat}Zn (between 1 and 5 Å) = 96.4 %



Simulated resonance for elements of interest(*)

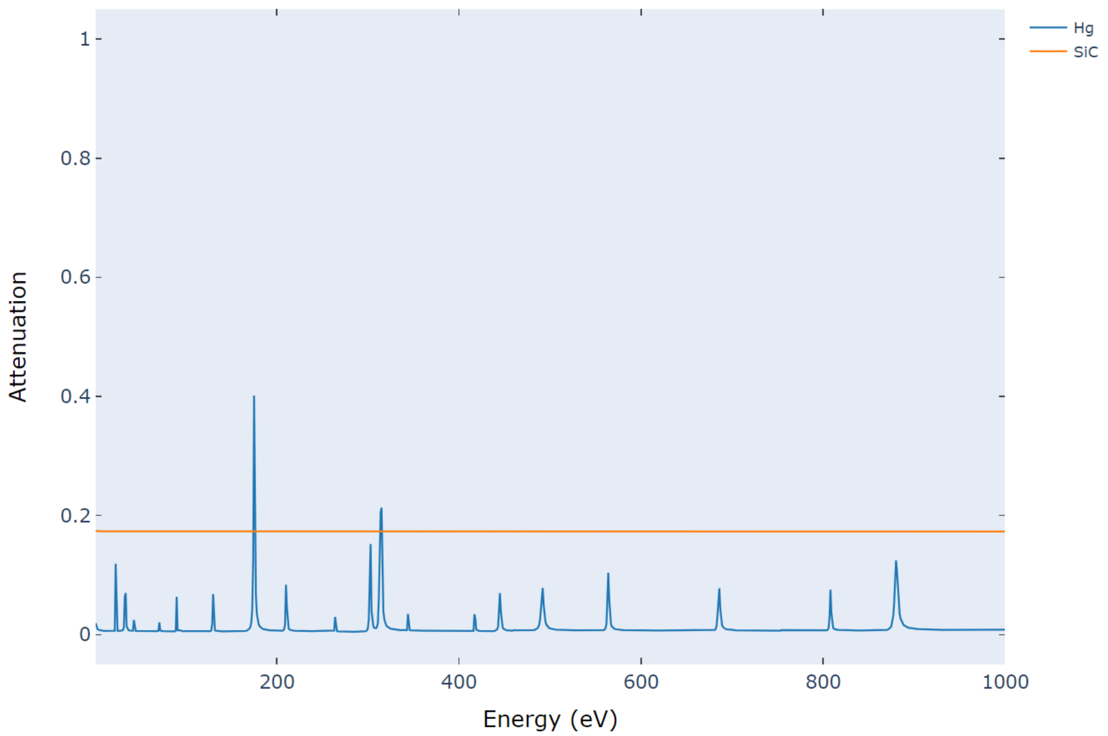




(*)Soil surveys in UK (1978-1983, 2000, 2011-2012)

Scientific applications that benefit from resonance imaging(cont'd)

- Hg contamination in soil
  - Assumptions: 0.1 mm Hg (13.6 g/cm^3) + 12.5 mm SiC (with 1.5 g/cm^3)
    - Transmission (1 and 5 Å) = 66.4 %



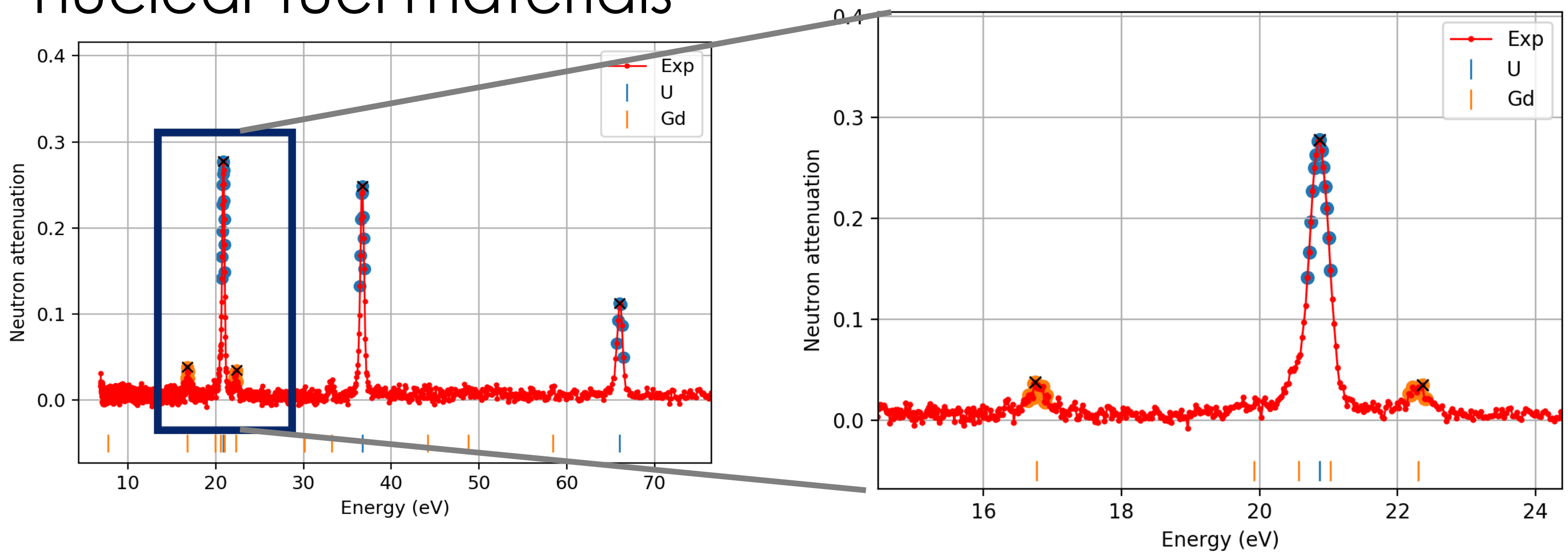
Resonance peaks plotted with:

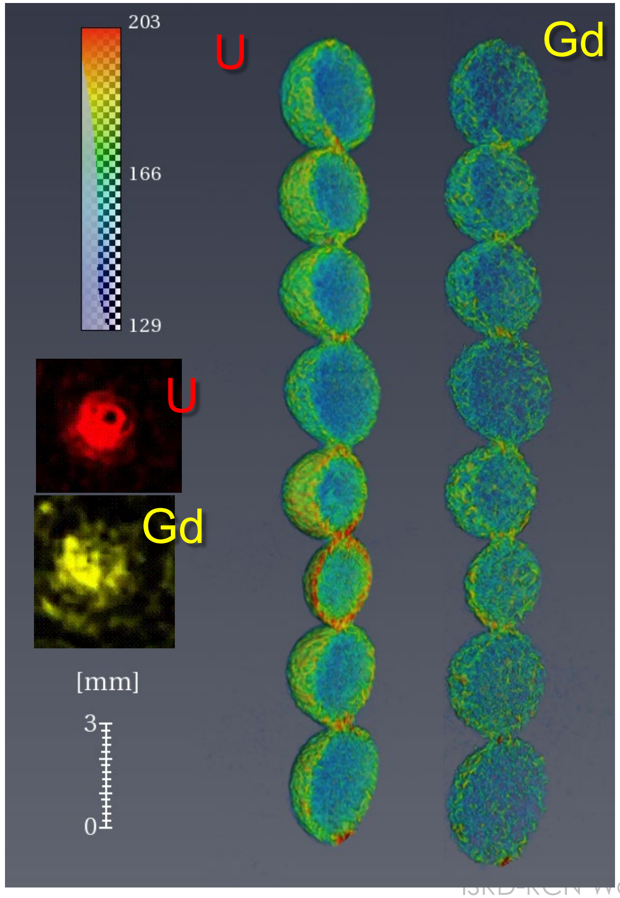
iNEUIT ("*I knew it*")

iNEUtron Imaging Toolbox

Using epithermal neutrons (energy > 1 eV), resonance imaging can map the isotopic content in advanced nuclear fuel materials in 3D

- ➢ Distribution of elements drive the performance of the novel advanced nuclear fuel materials





- ➢ **Quantitative analysis is being developed using in-house open-source Python package (ResoFit)**

Myhre K.G., Zhang Y., Bilheux H.Z., Johnson J.A., Bilheux J., Miskowiec A., Hunt R.D., "Nondestructive Tomographic Mapping of Uranium and Gadolinium Using Energy-Resolved Neutron Imaging", *Transactions of the American Nuclear Society,* (2018).

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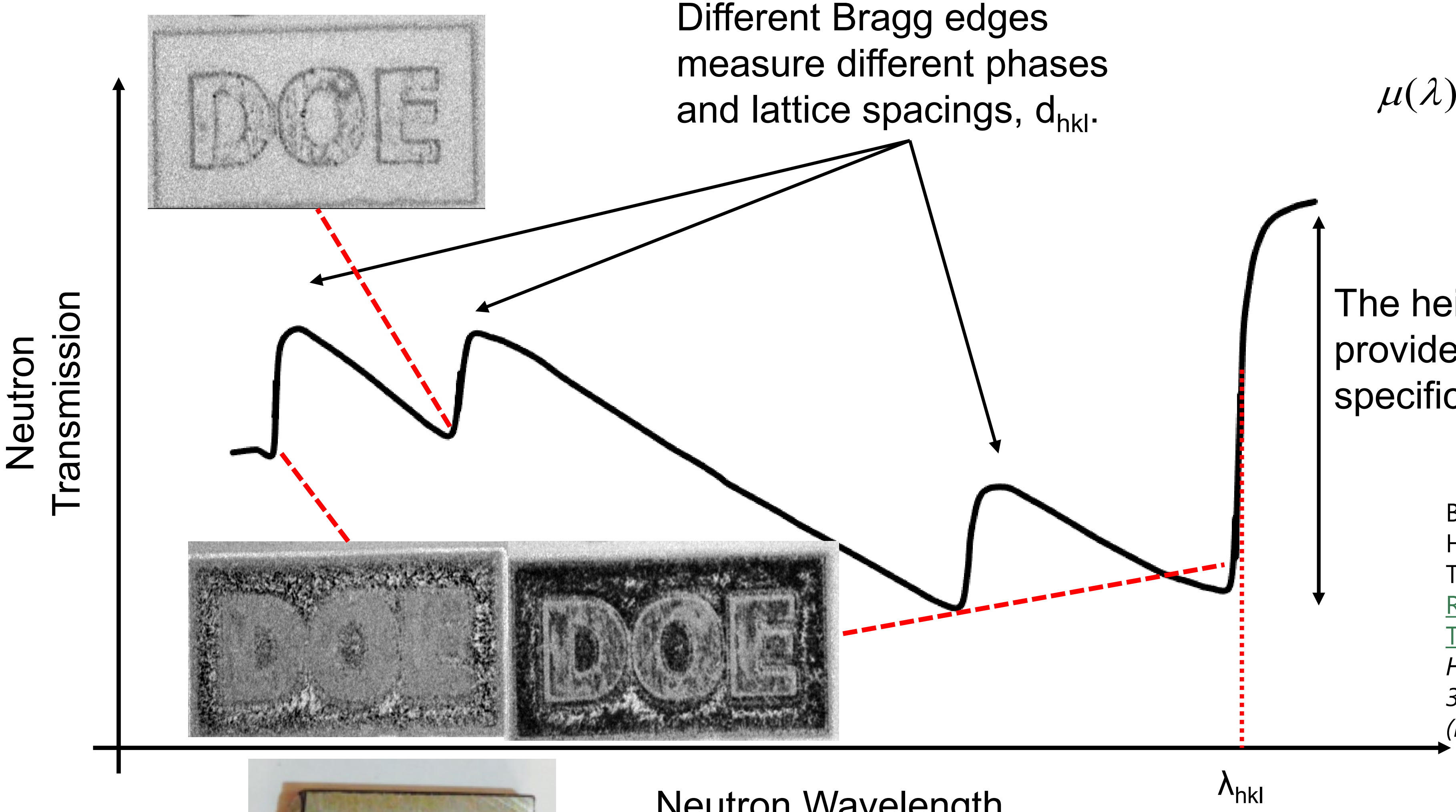
Bragg edge imaging: how does it work?

$$I(\lambda) = I_0(\lambda)e^{-\mu(\lambda)x}$$

$$\mu(\lambda) = \sigma_t(\lambda)\frac{\rho N_A}{M}$$

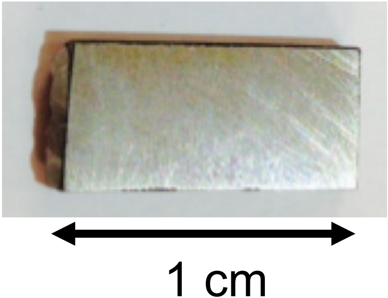
Different Bragg edges measure different phases and lattice spacings, d_{hkl}.



The height of Bragg edge provides the *amount* of a specific phase.

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).

3D printed Inconel 718



The position of the Bragg edge, **$\lambda_{hkl} = 2\ d_{hkl}$**, is a measure of the *strain* in the sample

Principle of Bragg edge Transmission

- ✓ Utilizes thermal and cold neutrons (approximately between 1 and 10 Å)
- ✓ Obeys Bragg's Law $\lambda_{hkl} = 2d_{hkl} \sin \theta_{hkl}$ simplifies: $\lambda_{hkl} = 2d_{hkl}$

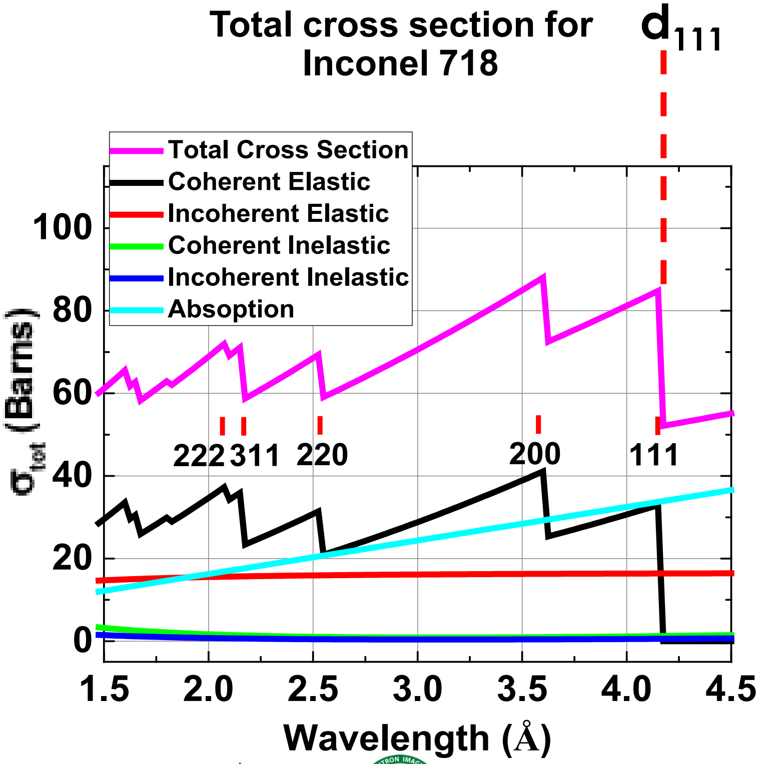
March-Dollase model

Sabine's primary extinction model

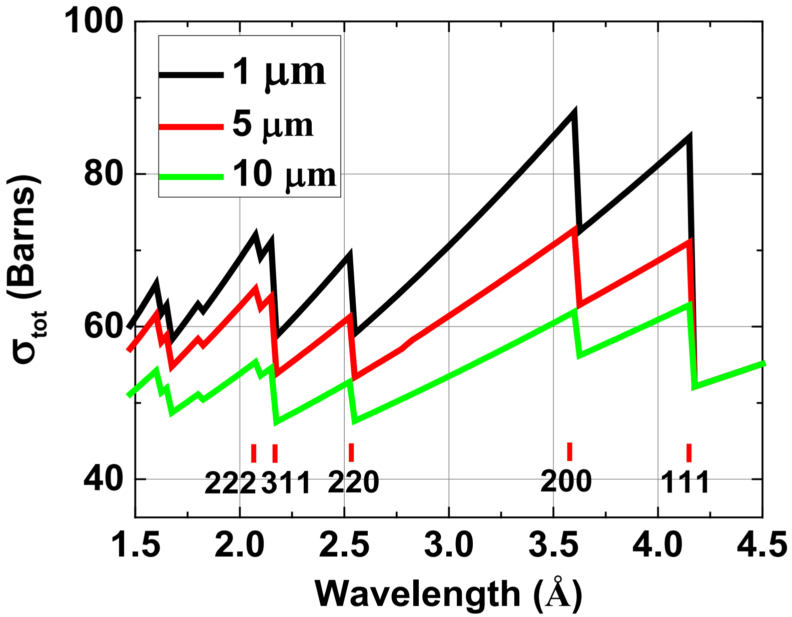
$$\sigma_{Bragg}(\lambda) = \frac{\lambda^2}{2V_0} \sum_{hkl}^{2d_{hkl}>\lambda} |F_{hkl}|^2 d_{hkl} \boxed{P\left(\alpha_{\vec{h}}(\lambda)\right)} \boxed{E_{hkl}(\lambda, F_{hkl})}$$

V_0: volume of unit cell
F_{hkl}: Structure factor including Debye-Waller factor

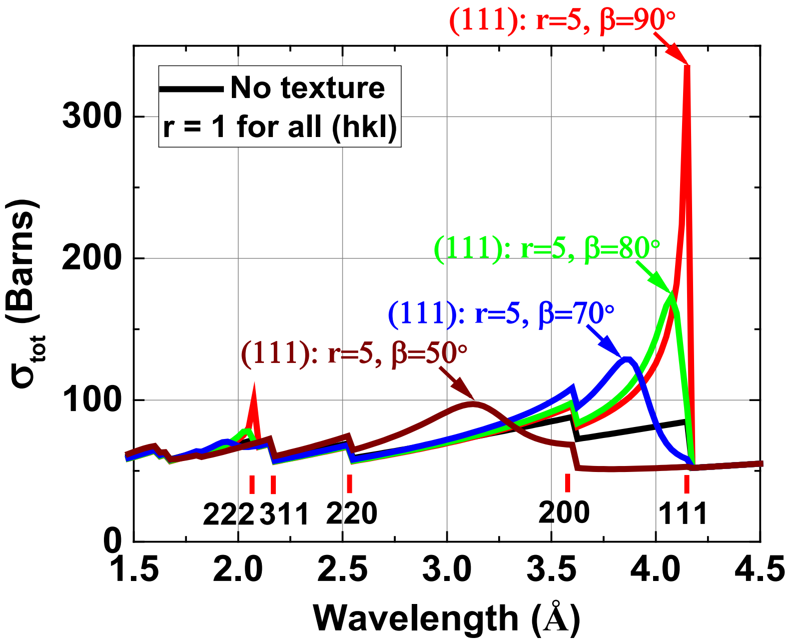
Total cross section for Inconel 718



Crystallite size effect (E_{hkl})

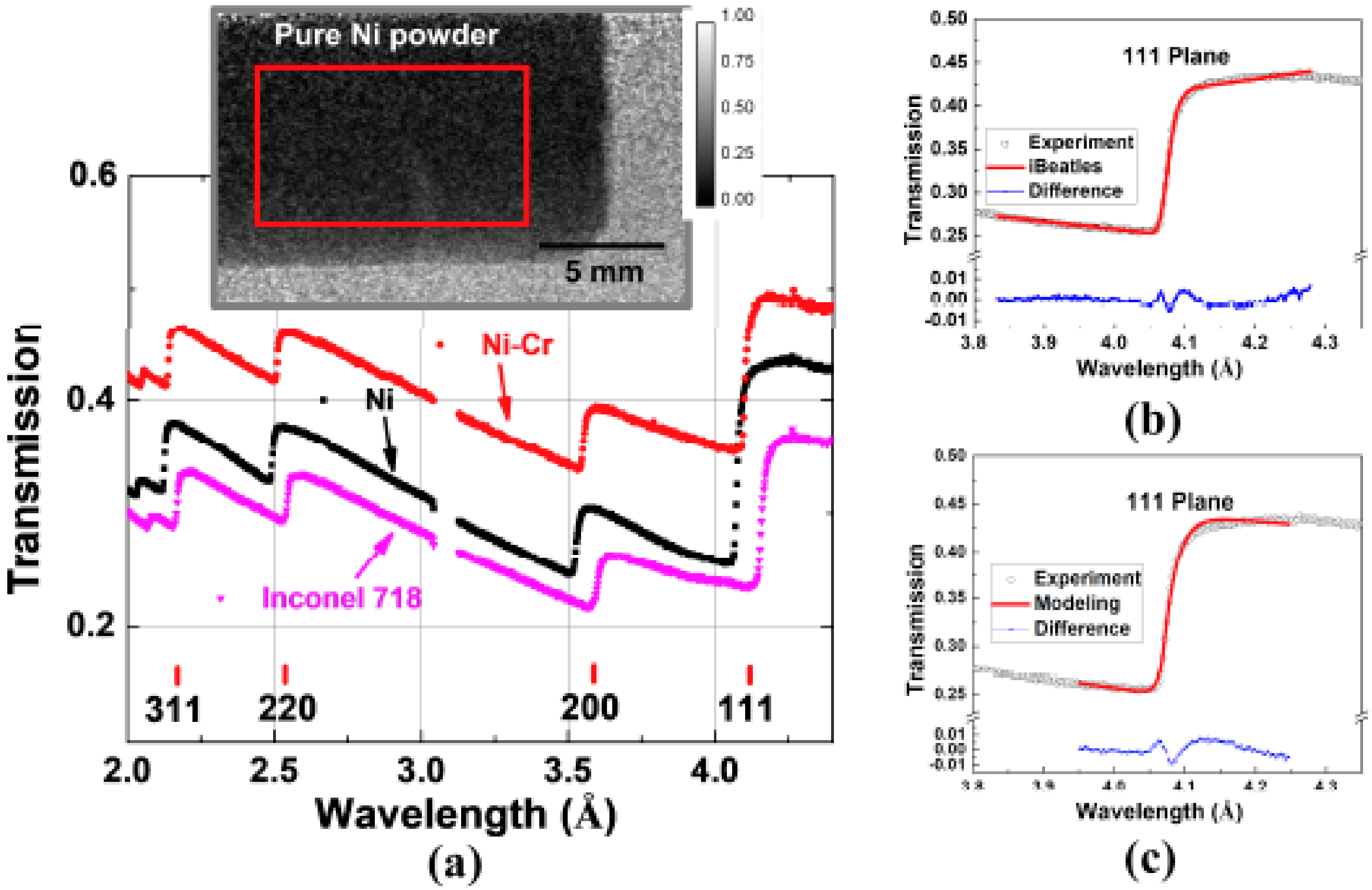


Crystallite orientation effect ($P\left(\alpha_{\vec{h}}(\lambda)\right)$: r and β)



G. Song et al., Journal of Imaging, 3, 65 (2017).

The perfect case study: powders



Song G., Lin J.Y., Bilheux J., Xie Q., Santodonato L., Molaison J.J., Skorpenske H.D., dos Santos A.M., Tulk C.A., An K., Stoica A.D., Kirka M.M., Dehoff R.R., Tremsin A.S., Bunn J.R., Sochalski-Kolbus L.M., Bilheux H.Z., "Characterization of Crystallographic Structures Using Bragg-Edge Neutron Imaging at the Spallation Neutron Source", *Journal of Imaging*, **3,** 4, 65 (2017).

Materials Behavior: Monitoring residual strain relaxation and preferred grain orientation of additively manufactured Inconel 625 by in-situ neutron imaging

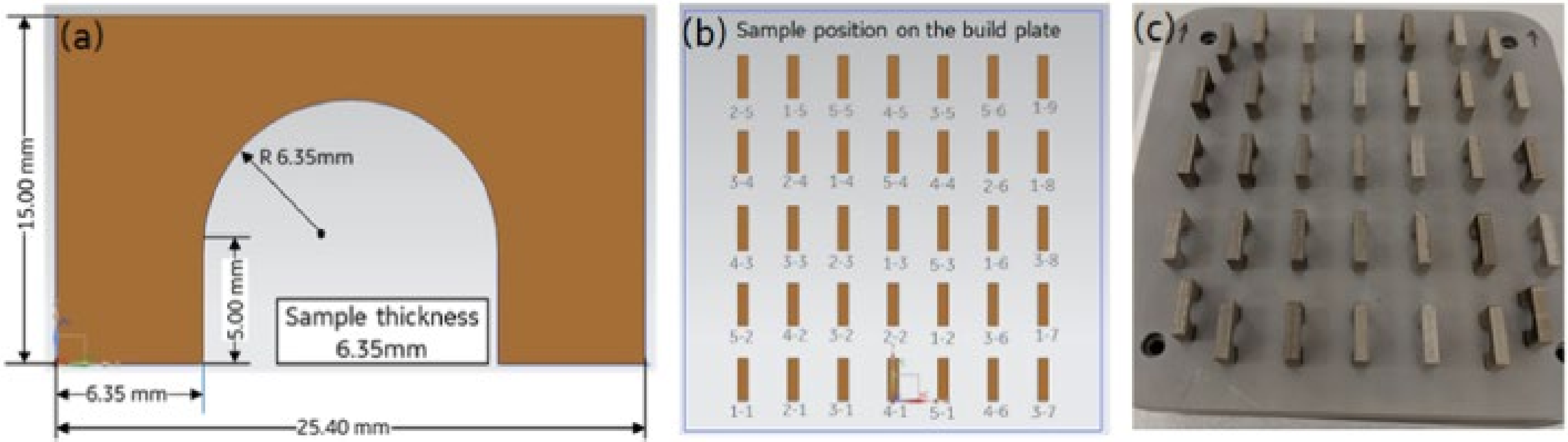
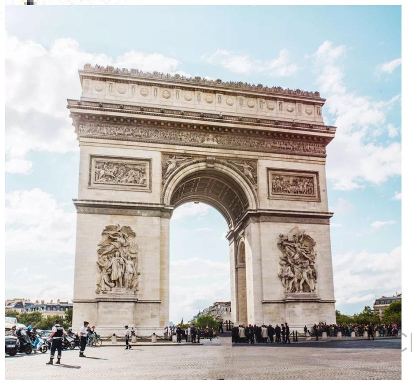


Fig. 1. (a) Sample design, (b) numbering and (c) the printed sample distribution on the build plate.

Tremsin et al, Additive Manufacturing, 2021.

Arc of Triumph, Paris.



https://www.tripsavvy.com/the-arc-de-triomphe-in-paris-1618623

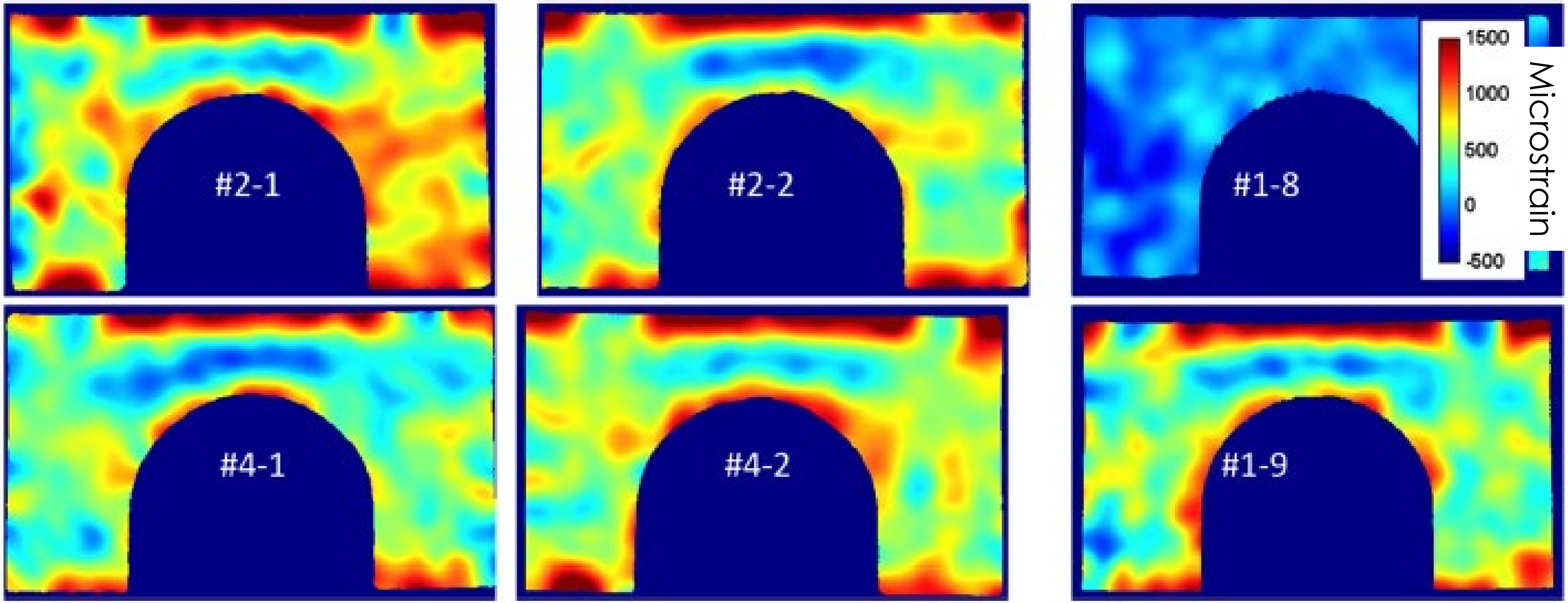
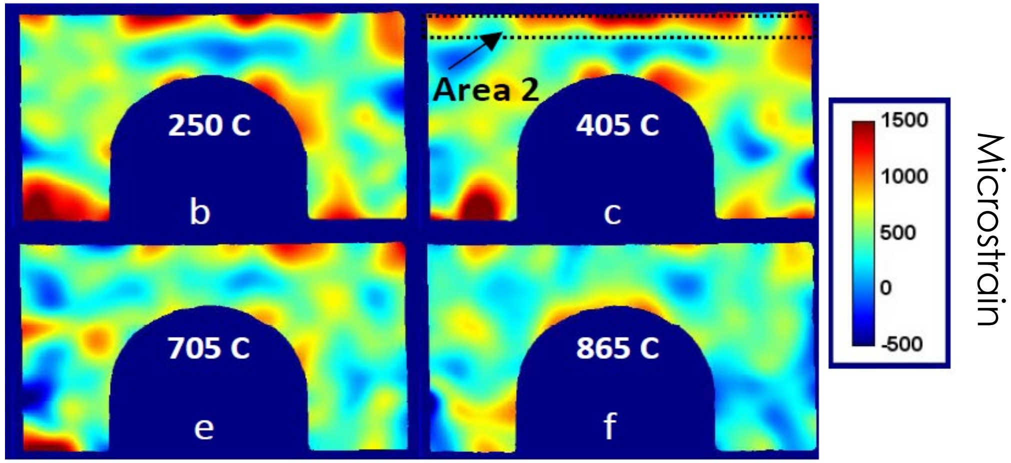
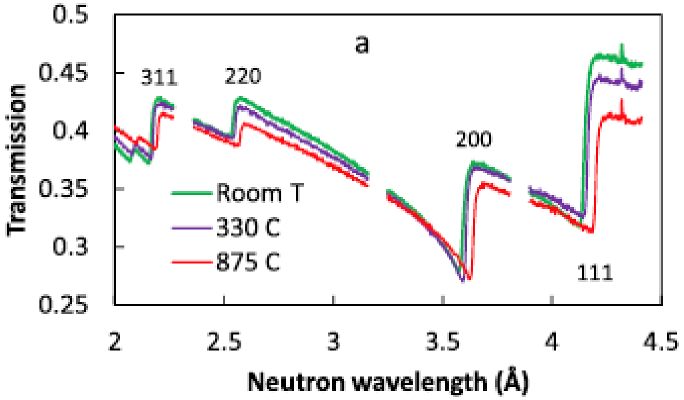


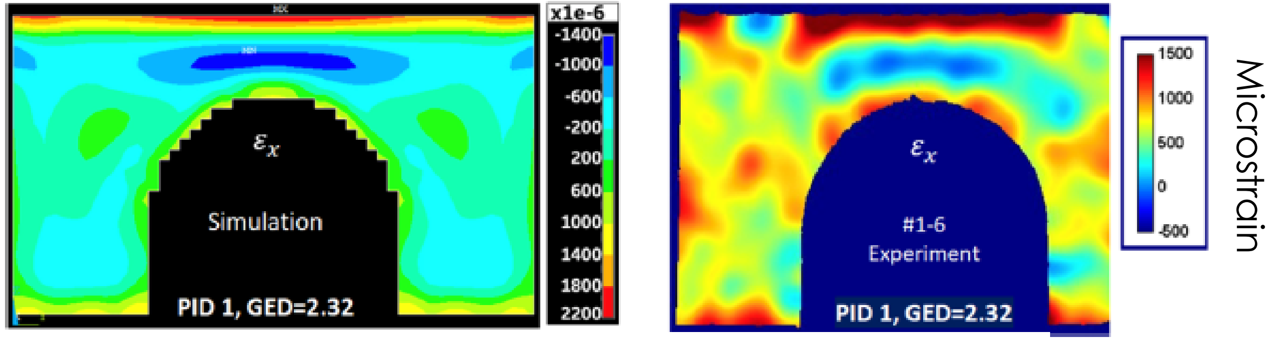
Fig. 8. Strain distribution (in microstrain) at the (111) Bragg edge measured at room temperature along the sample thickness direction X. SNAP beamline. The image integration time was about 2 h at SNAP. λ_0 value is taken from the annealed sample #1–8 (average across the entire sample). The legend indicates the strain values in microstrain.

Engineered Materials: Monitoring residual strain relaxation and preferred grain orientation of additively manufactured Inconel 625 by in-situ neutron imaging (10 min measurements)



AM Inconel 625 strain evolution as a function of temperature





Modeled and experimental results.

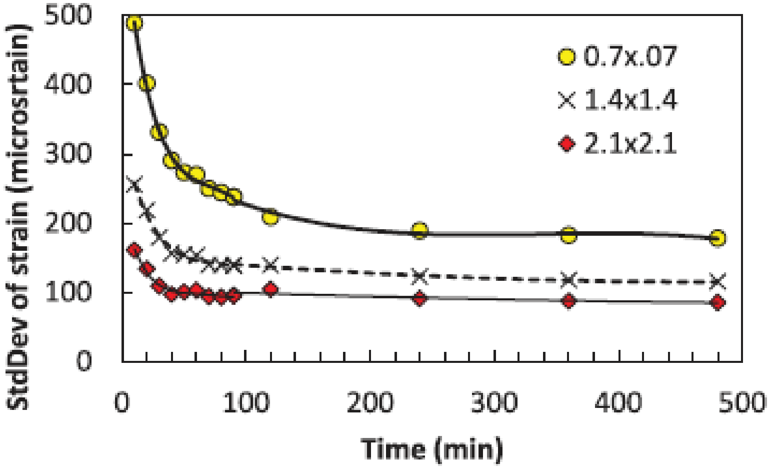


Fig. 16. Variation of the standard deviation of the reconstructed strain as a function of image integration time. Three different sizes of the area used for pixel grouping are used for strain reconstruction, as indicated by the legend (in mm^2).

Tremsin et al, Additive Manufacturing, 2021.

Tremsin et al, Nuc. Instr. Methods in Phys. Res. A, 2021.

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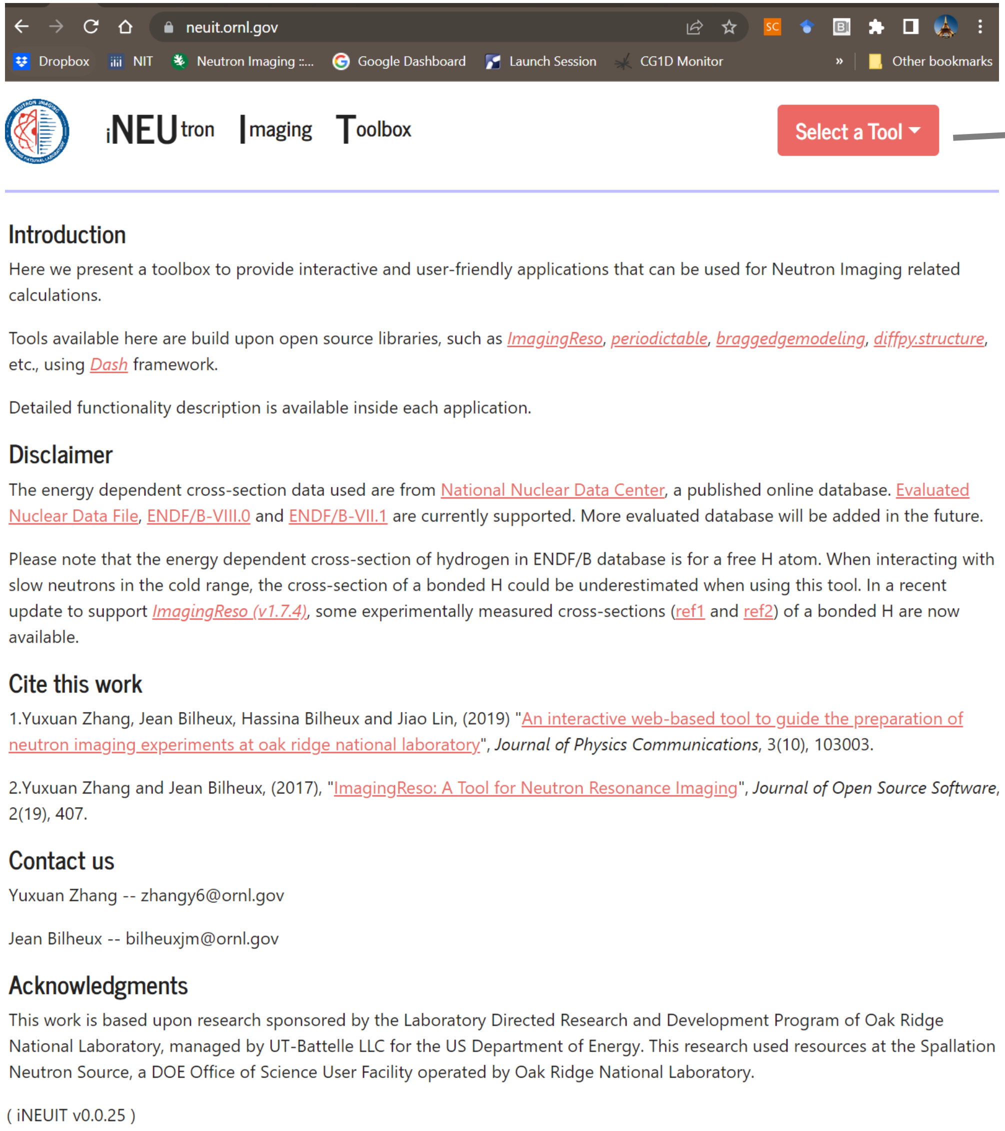
Experiment planning tools: *NEUIT* (**NEU**tron **I**maging **T**oolbox)



Introduction

Here we present a toolbox to provide interactive and user-friendly applications that can be used for Neutron Imaging related calculations.

Tools available here are build upon open source libraries, such as *ImagingReso*, *periodictable*, *braggedgemodeling*, *diffpy.structure*, etc., using *Dash* framework.

Detailed functionality description is available inside each application.

Disclaimer

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.

Please note that the energy dependent cross-section of hydrogen in ENDF/B database is for a free H atom. When interacting with slow neutrons in the cold range, the cross-section of a bonded H could be underestimated when using this tool. In a recent update to support *ImagingReso (v1.7.4)*, some experimentally measured cross-sections (ref1 and ref2) of a bonded H are now available.

Cite this work

1.Yuxuan Zhang, Jean Bilheux, Hassina Bilheux and Jiao Lin, (2019) "An interactive web-based tool to guide the preparation of neutron imaging experiments at oak ridge national laboratory", *Journal of Physics Communications*, 3(10), 103003.

2.Yuxuan Zhang and Jean Bilheux, (2017), "ImagingReso: A Tool for Neutron Resonance Imaging", *Journal of Open Source Software*, 2(19), 407.

Contact us

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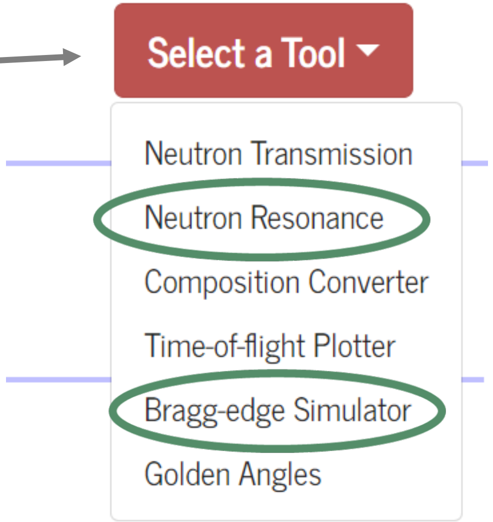
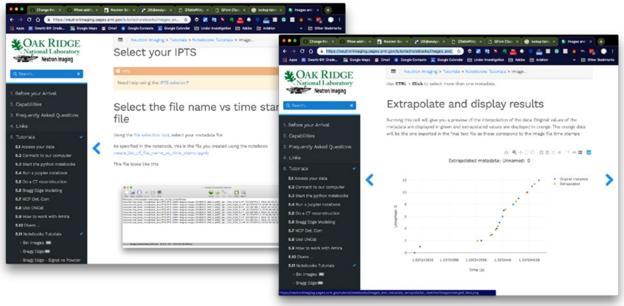
(iNEUIT v0.0.25)

- Available tools:



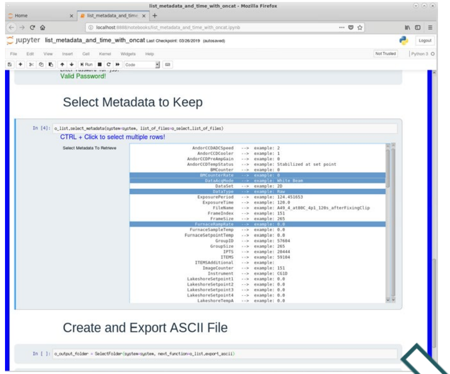
- Nuclear database supported
  - ENDF/B-VIII.0 (BNL)
  - ENDF/B-VII.1 (BNL)
- Elemental/isotopic info
  - PeriodicTable 1.5.0 (NIST)

We use Jupyter python notebooks developed to process/analyze data

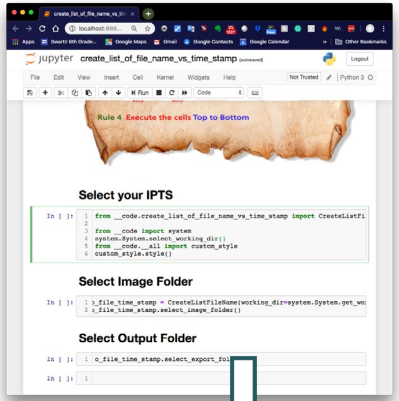


Scientific Achievement

Users can easily match metadata recorded with their own hardware to the corresponding image file.



Create lookup table of
Filename vs archived metadata



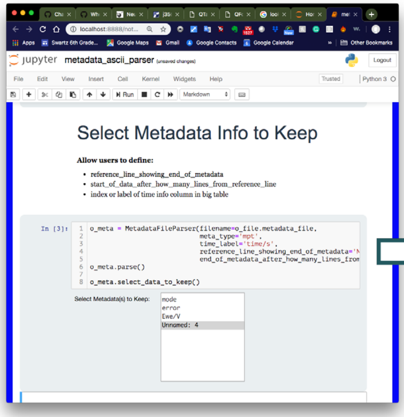
Create lookup table
filename vs timestamp

Significance and Impact

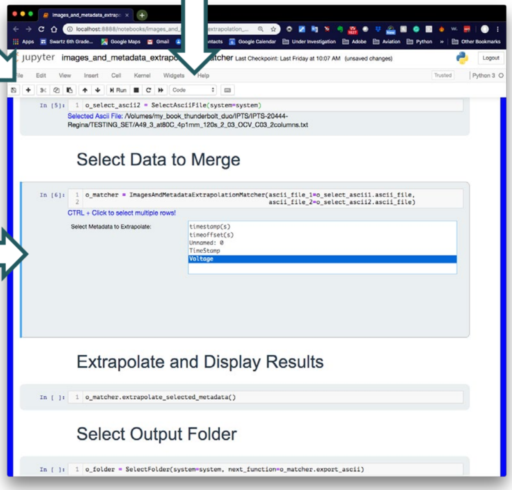
– In any experiments, parameters are modified, monitor and recorded. Those metadata are sometimes store with the image file, archived or just saved in an external text file. This notebook allows to bring all those metadata into a single place in order to match them with the right file.

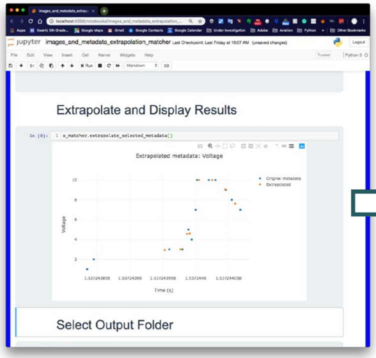
Research Details

– A first notebook create a lookup table of file name vs time stamp. According to the location of the metadata, another notebook is ran to create this time a lookup table of metadata vs time stamp. This 3rd notebook, presented here, allows to match or interpolate the correct metadata value for each image file.

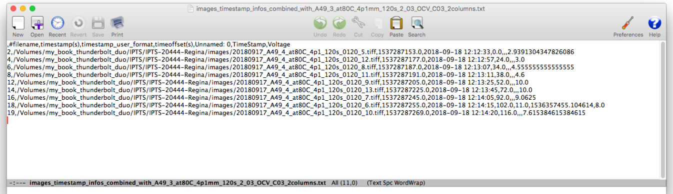


Create lookup table of
Metadata vs timestamp





This notebook showing the result of the interpolated metadata.

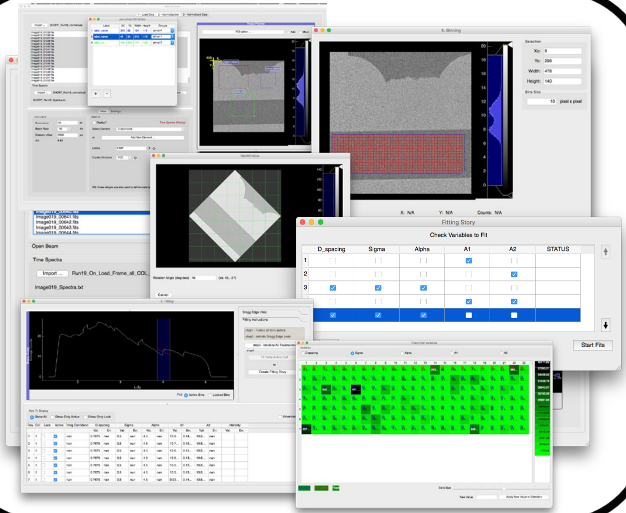


Lookup table of **filename vs metadata vs timestamp**

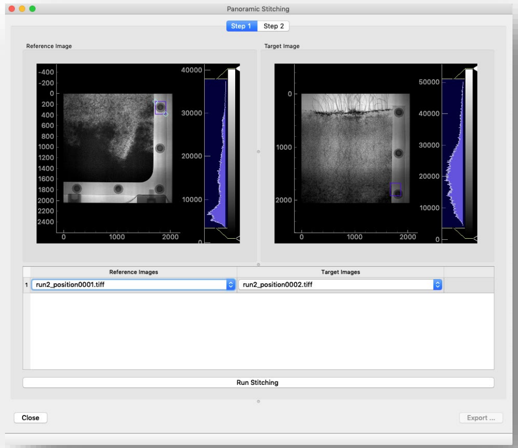
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE | NEUTRON IMAGING

Advanced tasks

Bragg Edge

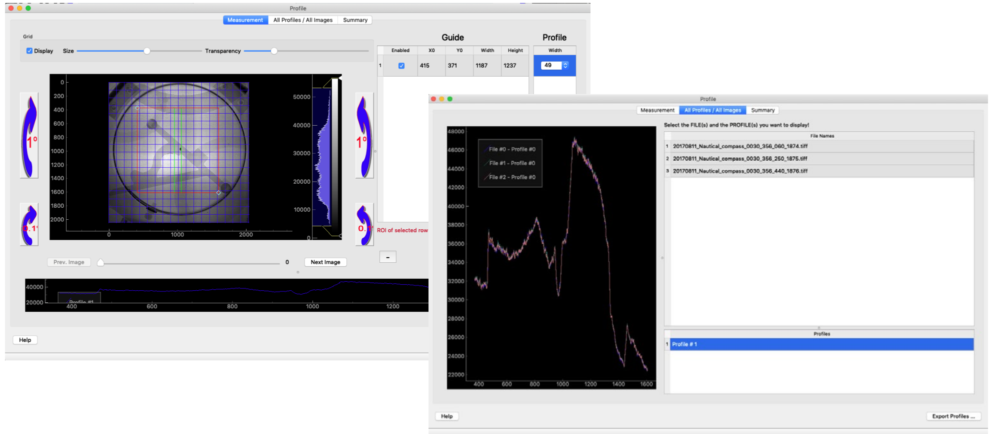


Panoramic Stitching



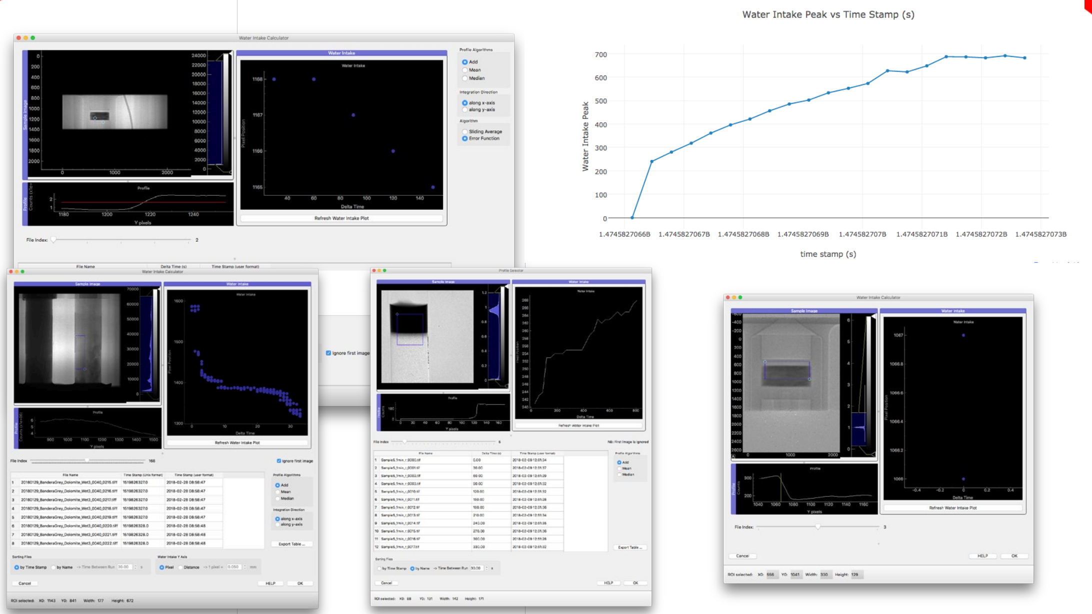
Cylindrica

Water-intake profile Calculator

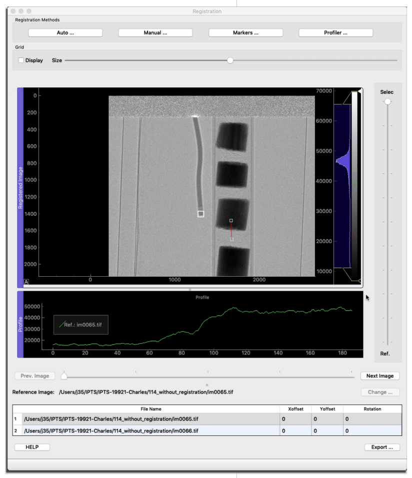


GitHub https://github.com/ornlneutronimaging/CylindricalGeometryCorrection

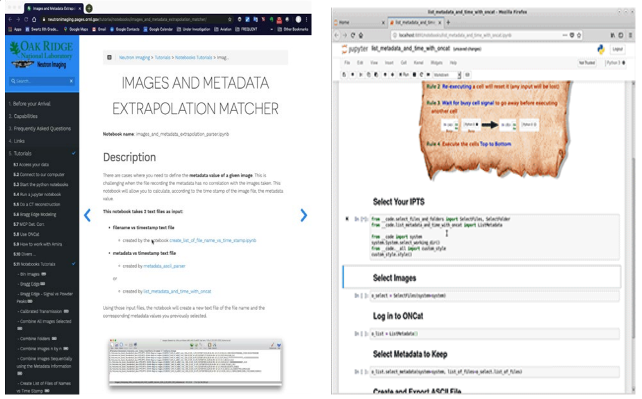
Water-intake Profile Calculator



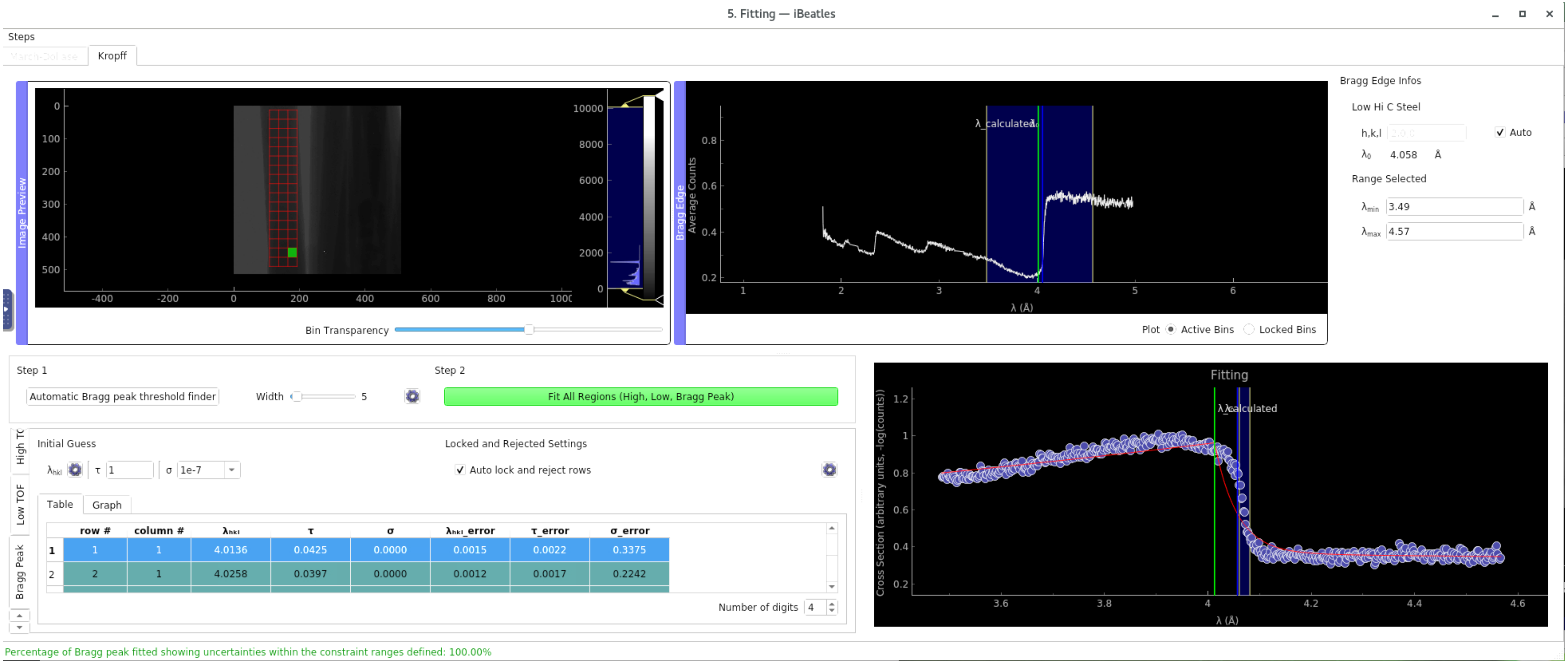
Registration



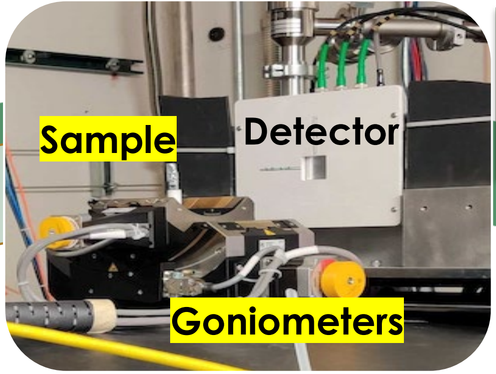
Images and Metadata Extrapolation Matcher



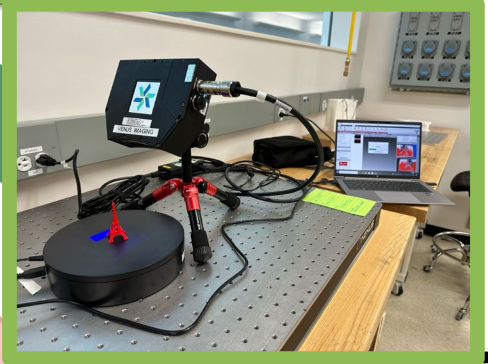
ORNL iBeatles software fits experimental Bragg edges

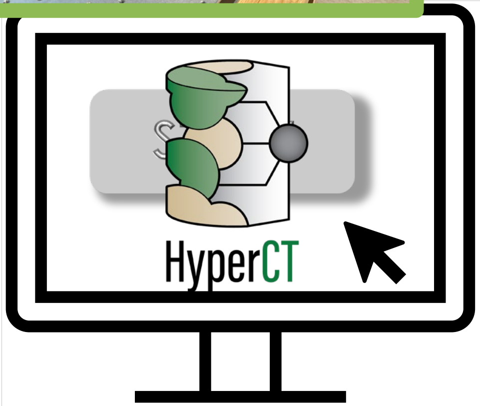


Autonomous Hyperspectral Neutron CT Experiment at ORNL



Light scan and preselection of projection angles





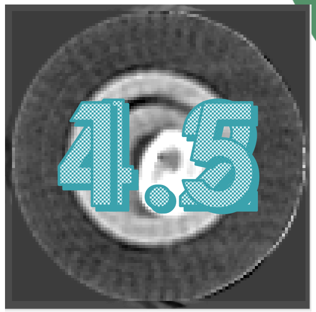
Continue

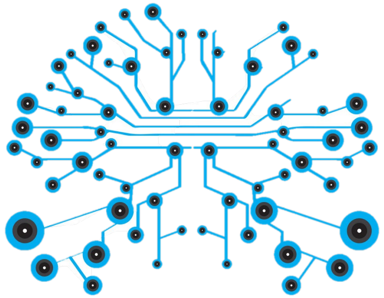
Stop

Autonomous Decision

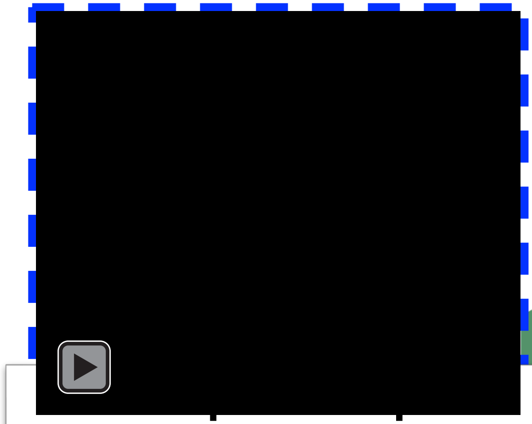
Up to factor 5 improvement in time

- Optimization of the scan based on the unique sample geometry
- Ability to provide real-time reconstructed data using advanced iterative reconstruction methods





AI Quality Evaluation



Scanning Angles (active learning)

Exciti
Intelli

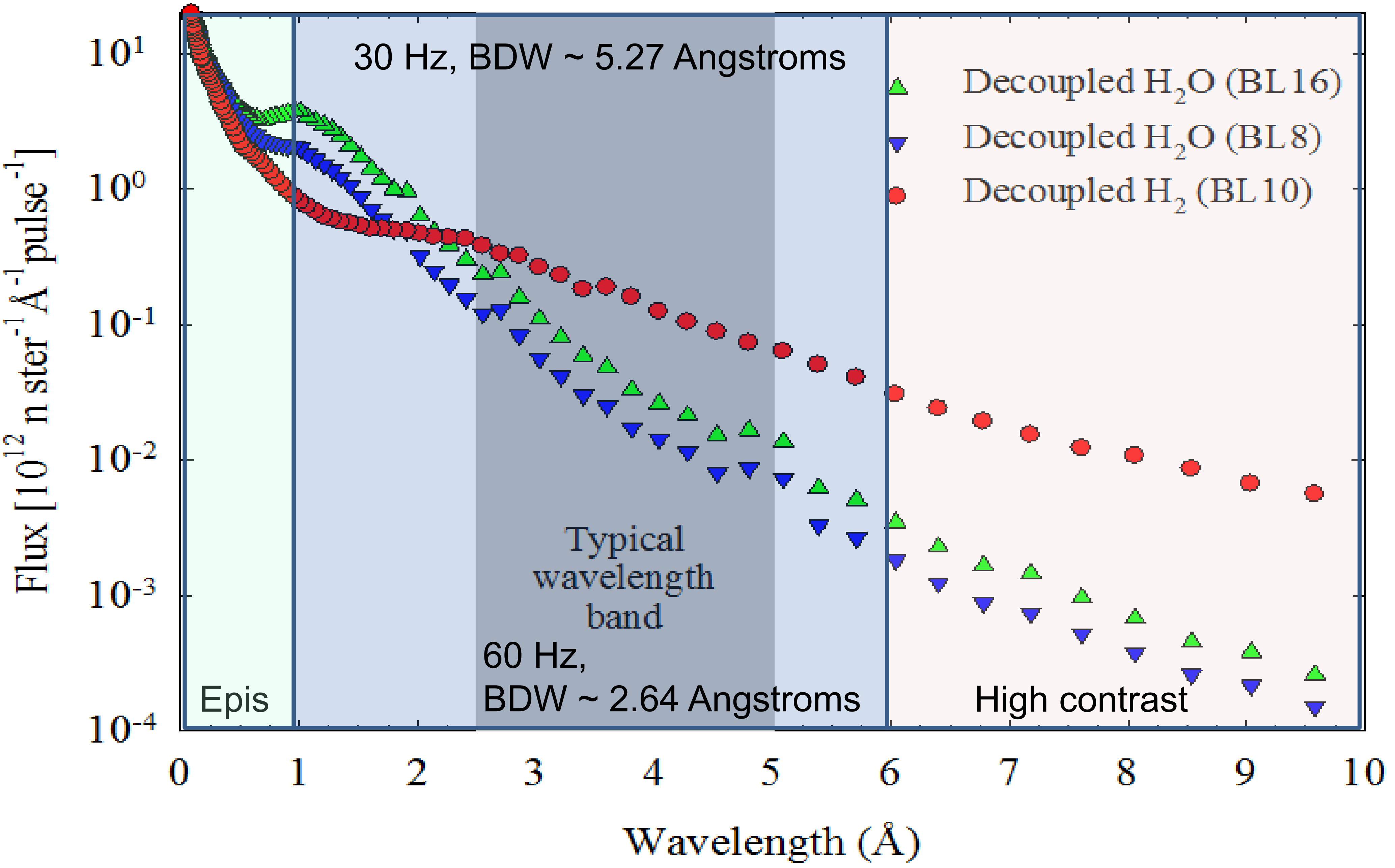

WALLY, I NEED YOU TO HEAD UP OUR ARTIFICIAL INTELLIGENCE PROJECT.
Dilbert.com
@ScottAdamsSays
YOU WILL HAVE NO BUDGET AND NO HOPE OF SUCCESS. I JUST LIKE SAYING WE'RE WORKING ON AI.
6-20-16 © 2016 Scott Adams, Inc. /Dist. by Universal Uclick
AND YOU'RE COMPLETELY USELESS, SO IT'S A GOOD MATCH.
I WON'T LET YOU DOWN.

Outline

- Neutron imaging facilities at ORNL
- Principle of time-of-flight (TOF) or hyperspectral neutron imaging
- Resonance imaging
- Bragg edge imaging
- Software efforts
- **VENUS**
- Conclusion

What is VENUS?

- VENUS is an imaging beamline that can measure unique materials properties based on their crystalline structures and isotopic content using two techniques:
  - **Bragg-edge imaging** – quantitative interpretation of total cross-section provides crystalline structure characterization (cold neutrons ~ meV)
  - **Resonance imaging** – isotopic-sensitive spatially-resolved spectroscopy technique (epithermal neutrons ~ eV)
- VENUS can also penetrate thicker samples using:
  - **Epithermal imaging** – higher energy neutrons provide higher penetration through thick samples (epithermal neutrons ~ eV)
- We are **developing hyperspectral reconstruction algorithms using machine learning algorithms** (due to low signal-to-noise ratio)



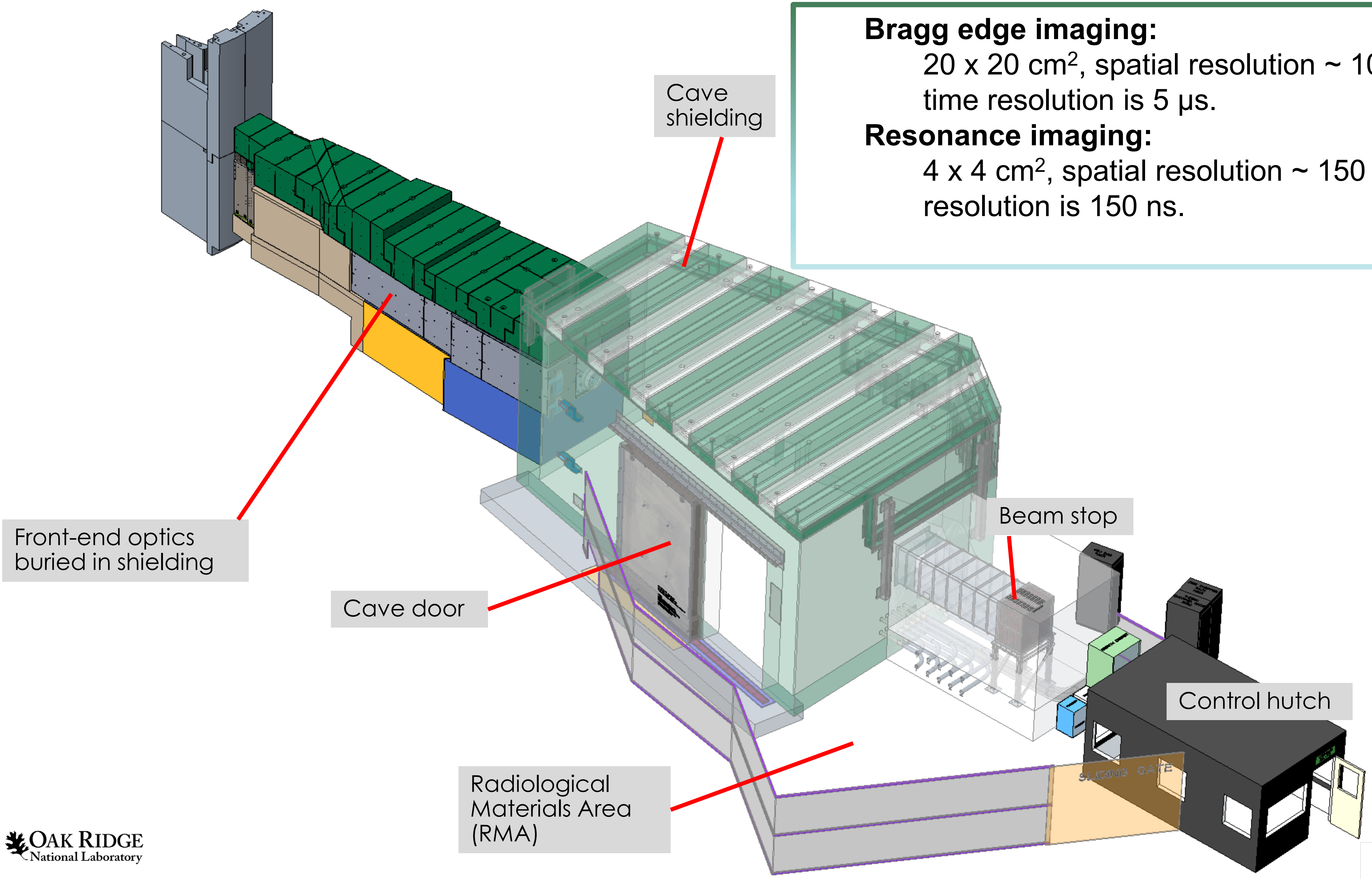
30 Hz, BDW ~ 5.27 Angstroms
Decoupled H2O (BL16)
Decoupled H2O (BL8)
Decoupled H2 (BL10)
Typical wavelength band
60 Hz,
BDW ~ 2.64 Angstroms
Epis
High contrast
Flux [10^12 n ster^-1 Å^-1 pulse^-1]
Wavelength (Å)
10^1
10^0
10^-1
10^-2
10^-3
10^-4
0 1 2 3 4 5 6 7 8 9 10

Bragg edge imaging:

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

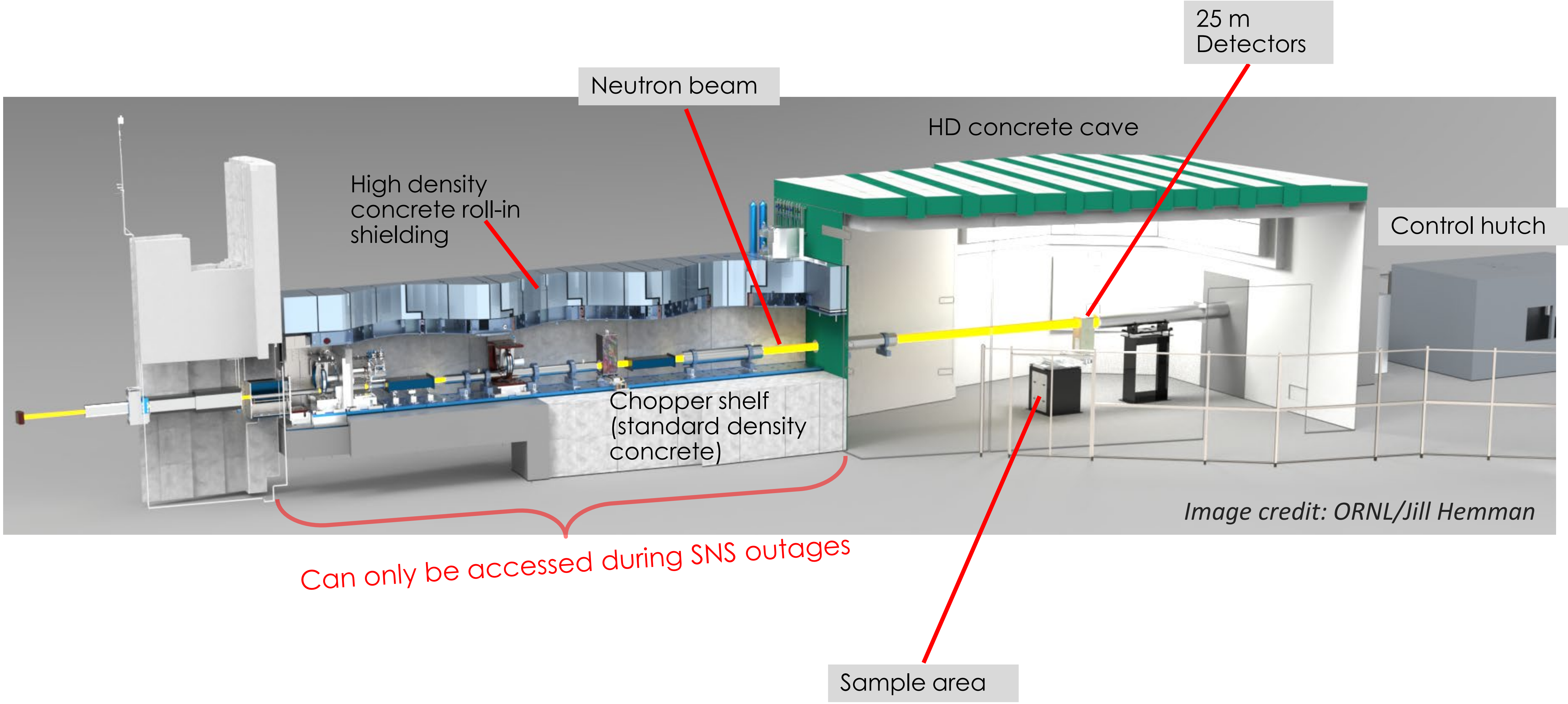
Resonance imaging:

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



Oak Ridge National Laboratory

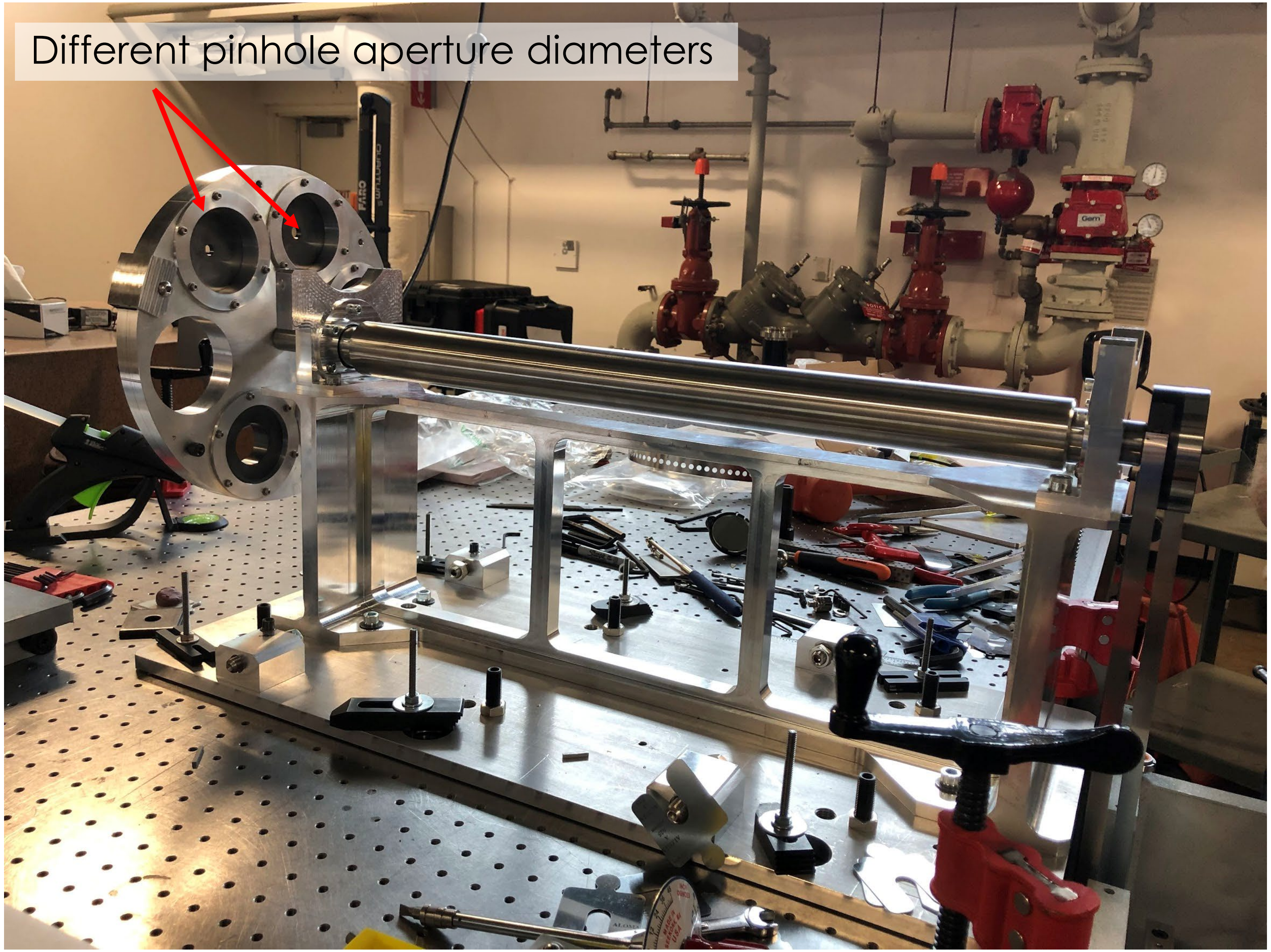
Artistic rendering of VENUS



VENUS Shutter, Core Vessel Insert and Fixed Aperture

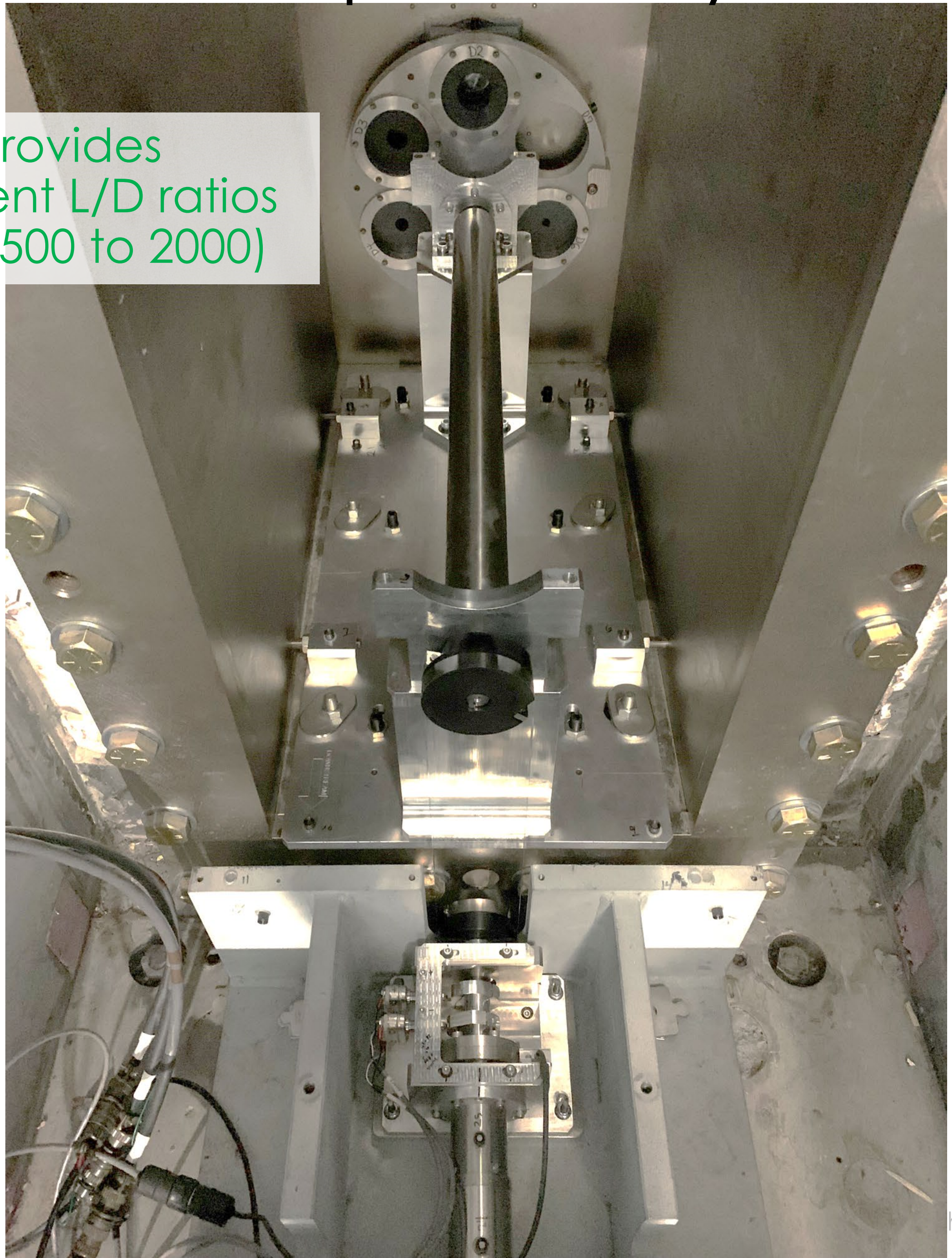
VENUS defining optics: variable aperture system (VAS)

- Installed 4.5 m away from the source
- Varies collimation ratio from 400 to 2000
- High collimation value:
  - Higher spatial resolution
  - Lower intensity
- Beam envelope goes from a circular to a square cross-section.

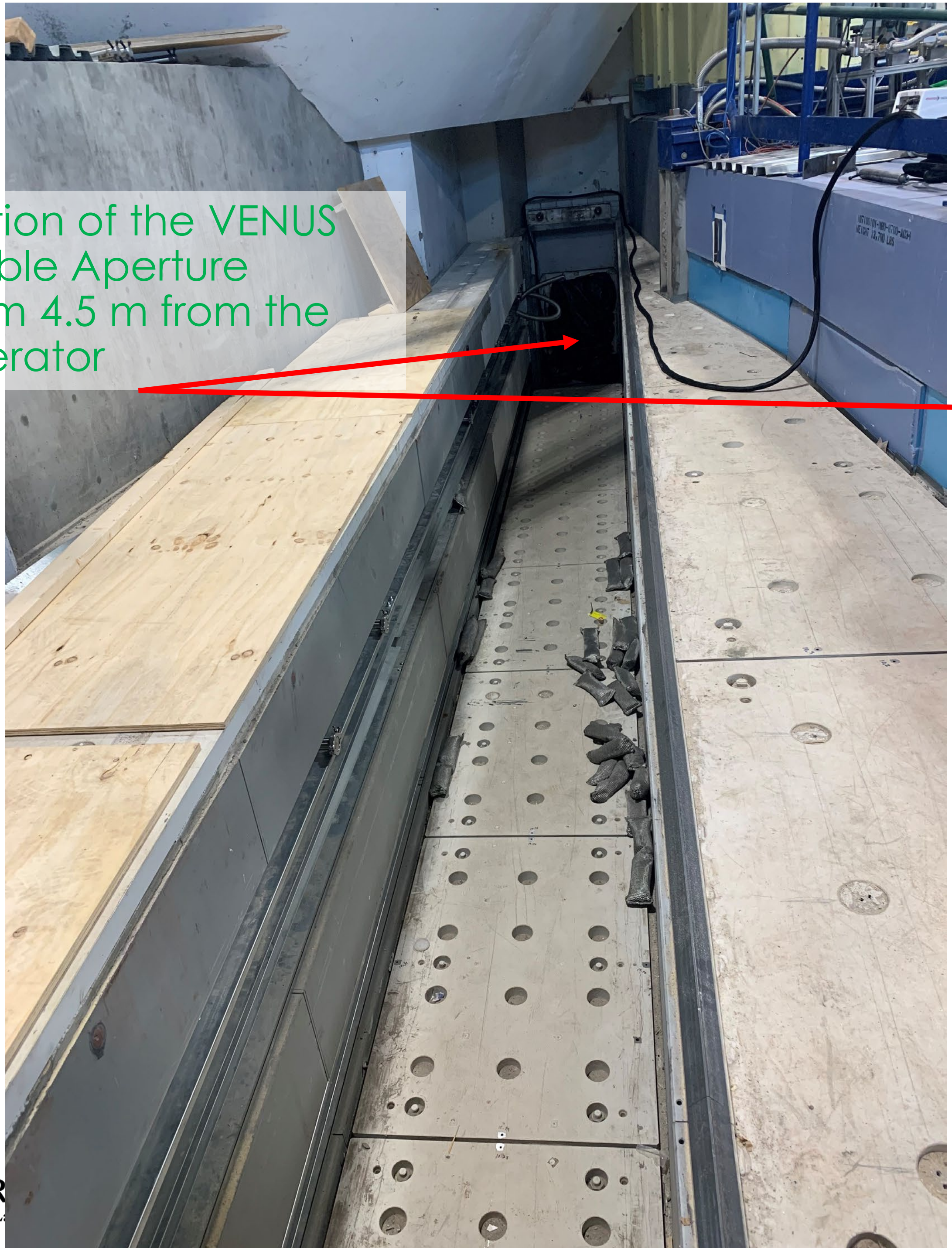


September 2022: Installation of Variable Aperture System

VAS provides different L/D ratios (from 500 to 2000)



Location of the VENUS Variable Aperture System 4.5 m from the moderator



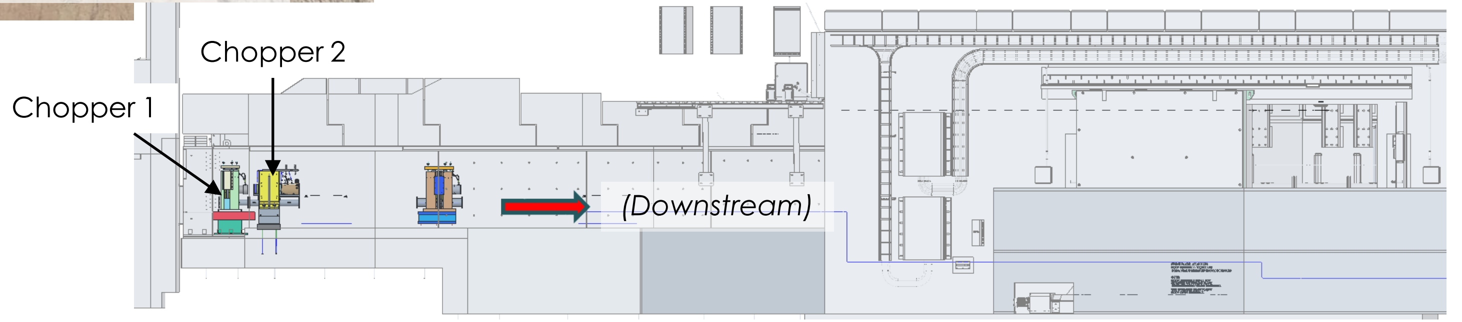
Trench is ~ 0.9 m wide

Chopper installation

Installed and tested Chopper 1

Installed and tested Chopper 2

Multiple cable pulls through-out instrument



Component shielding and flight tubes


Completed concrete pour for component shielding


Component Shielding Test Fit


Installed Flight Tube 2

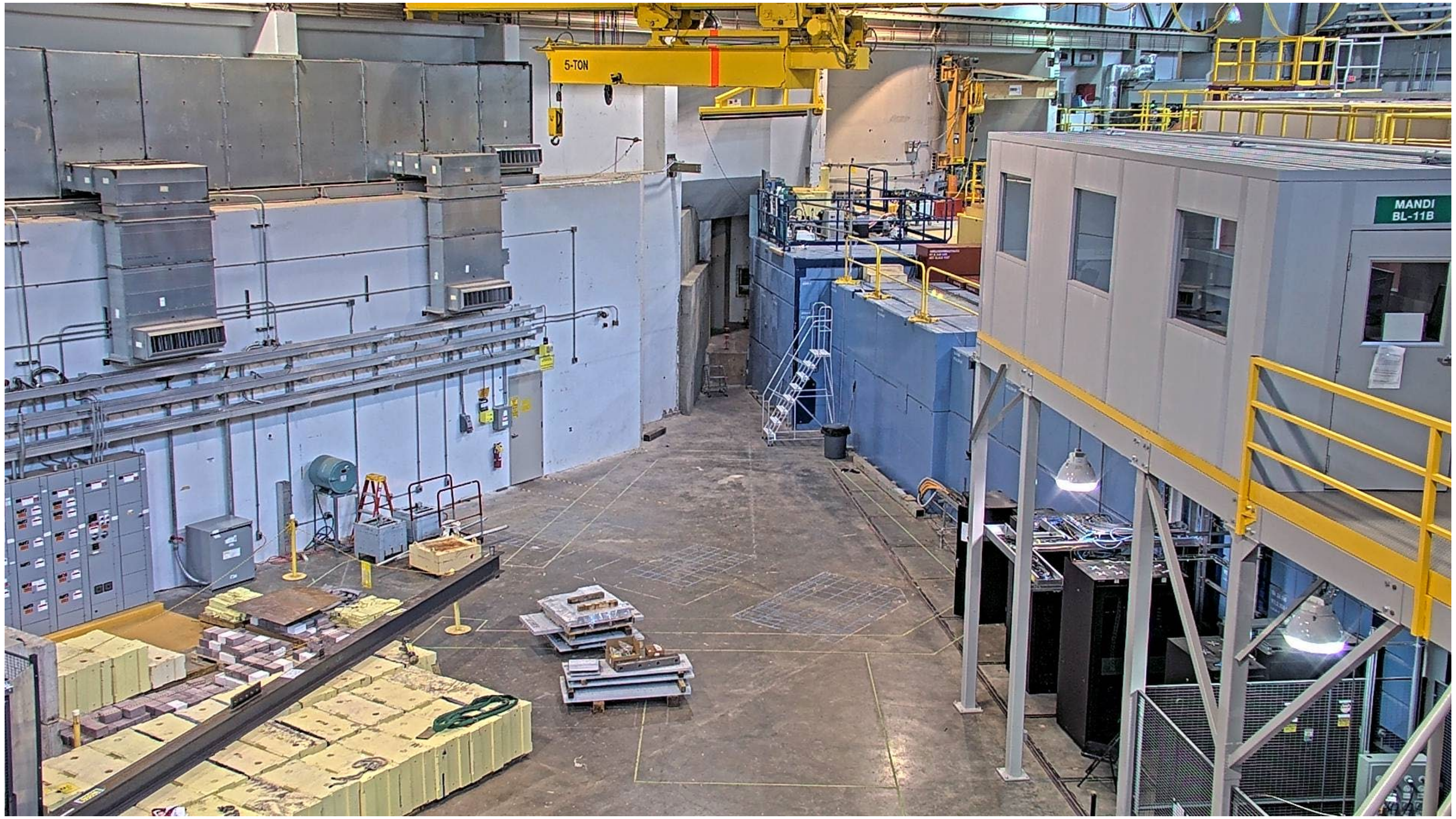
Installed Component Shielding

In the front end of the beamline:

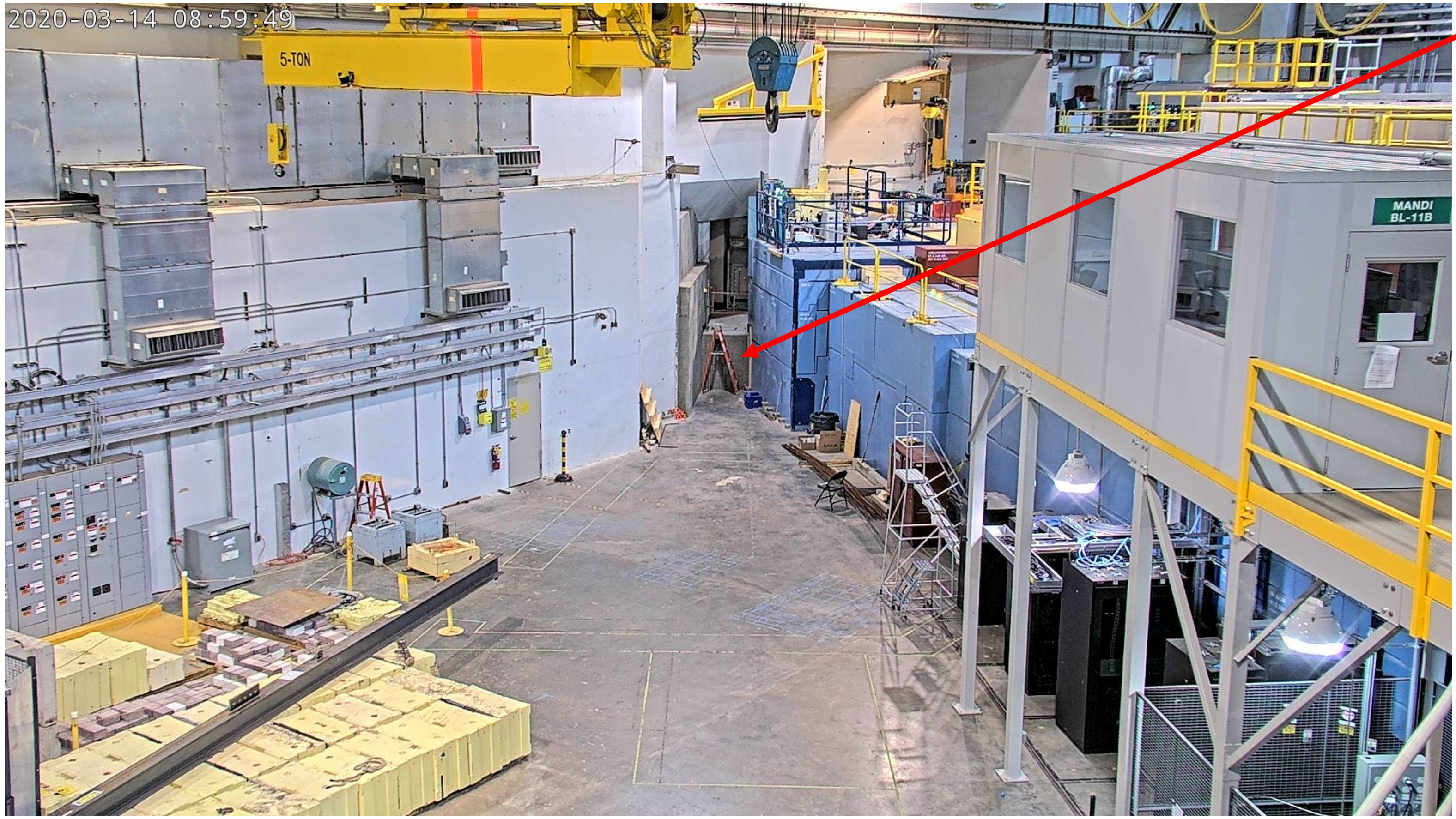
Green: Component shielding to reduce background in the VENUS cave

White: Configuration control shielding to protect personnel

February 2020

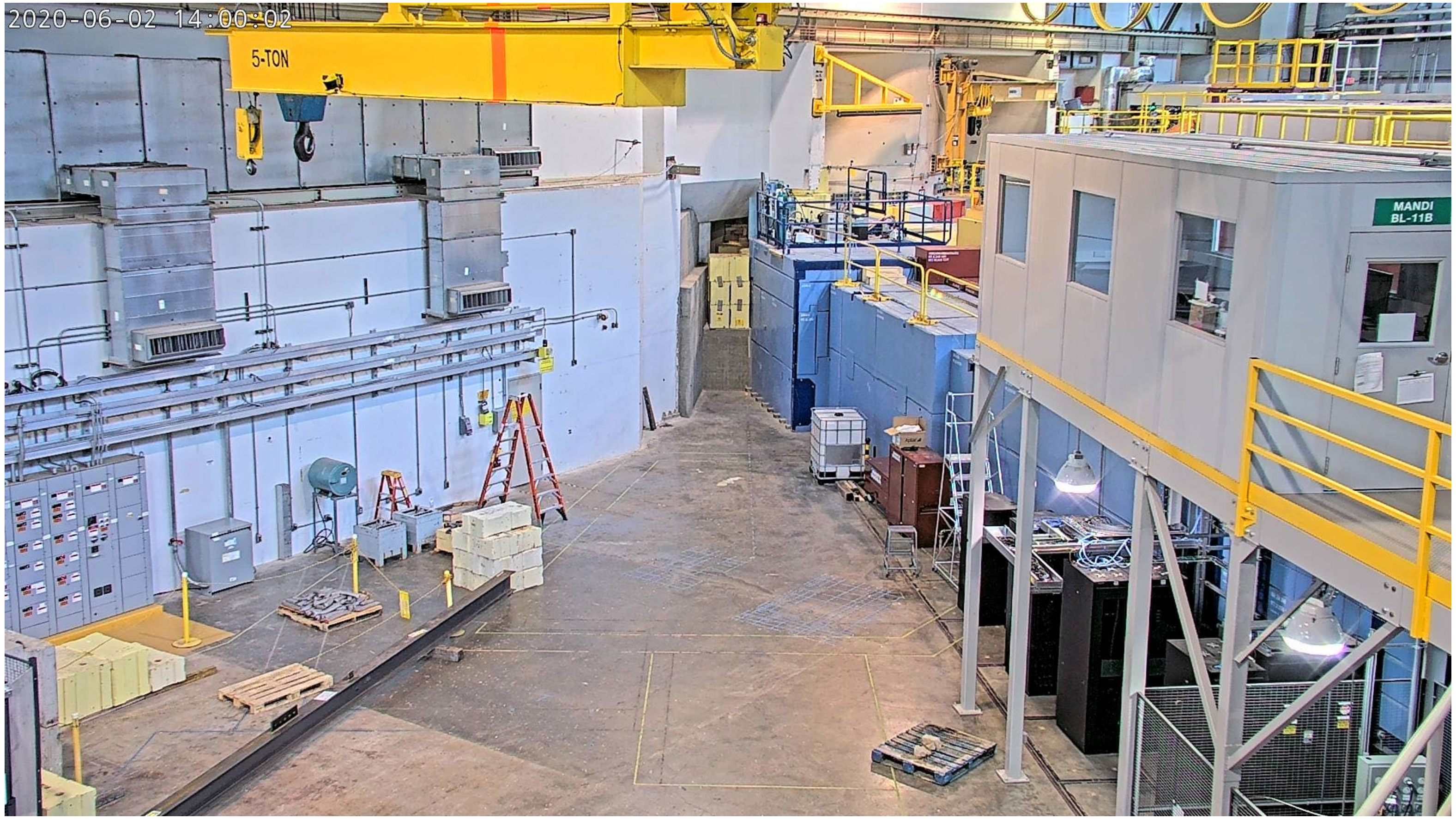


March 2020

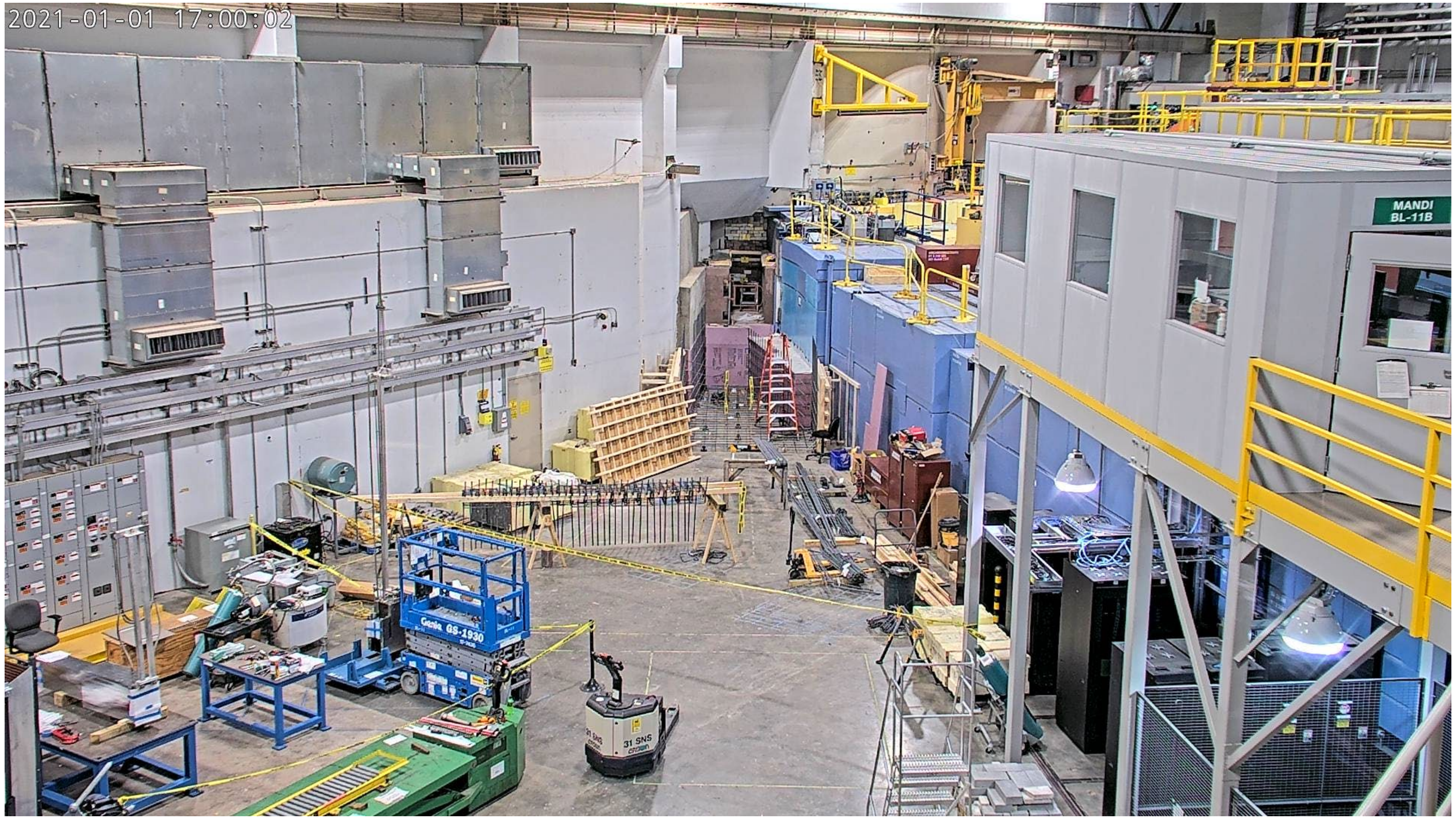


Started pouring the front-end shielding

June 2020

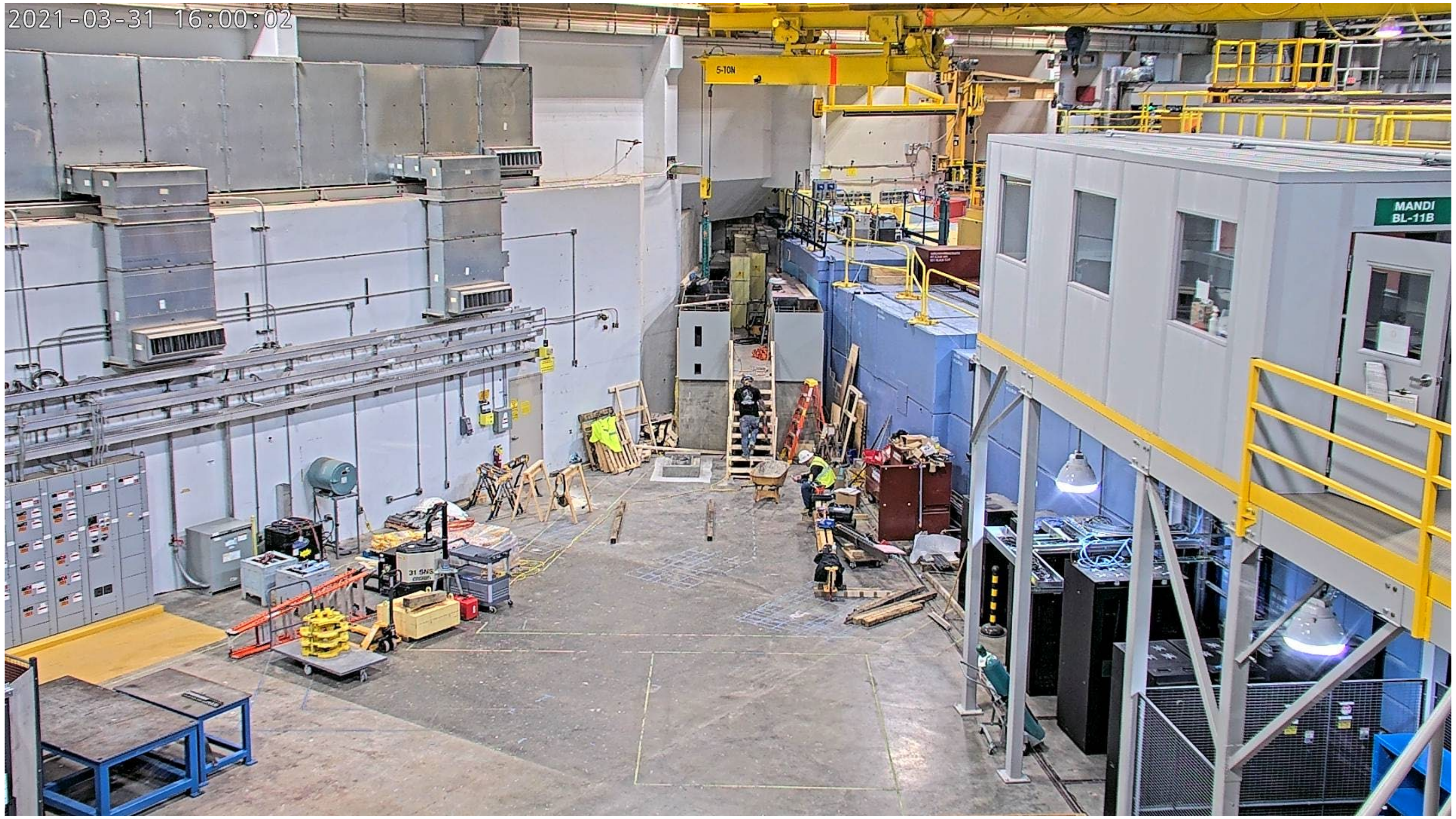


January 2021



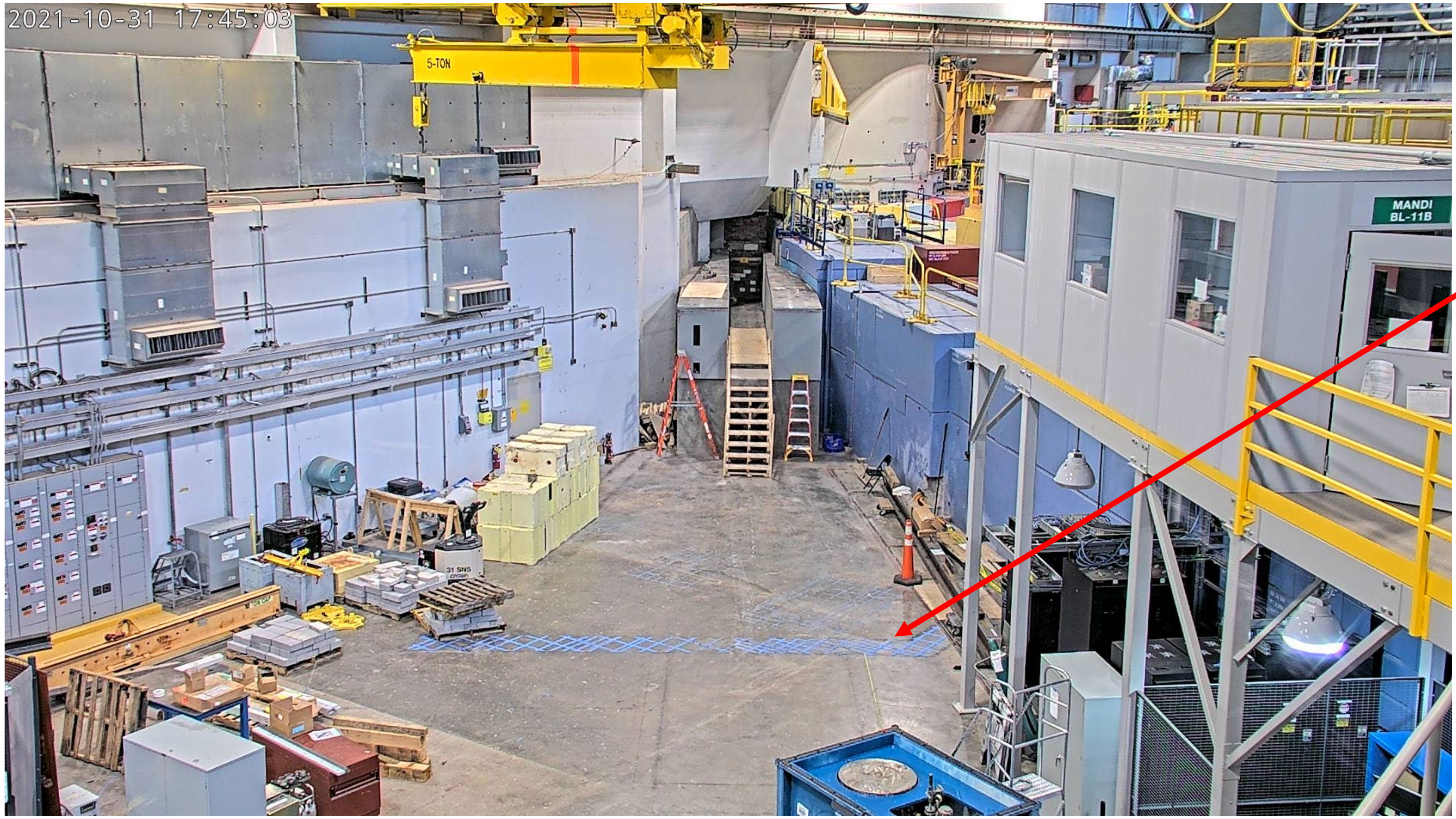
March 2021

March 2021



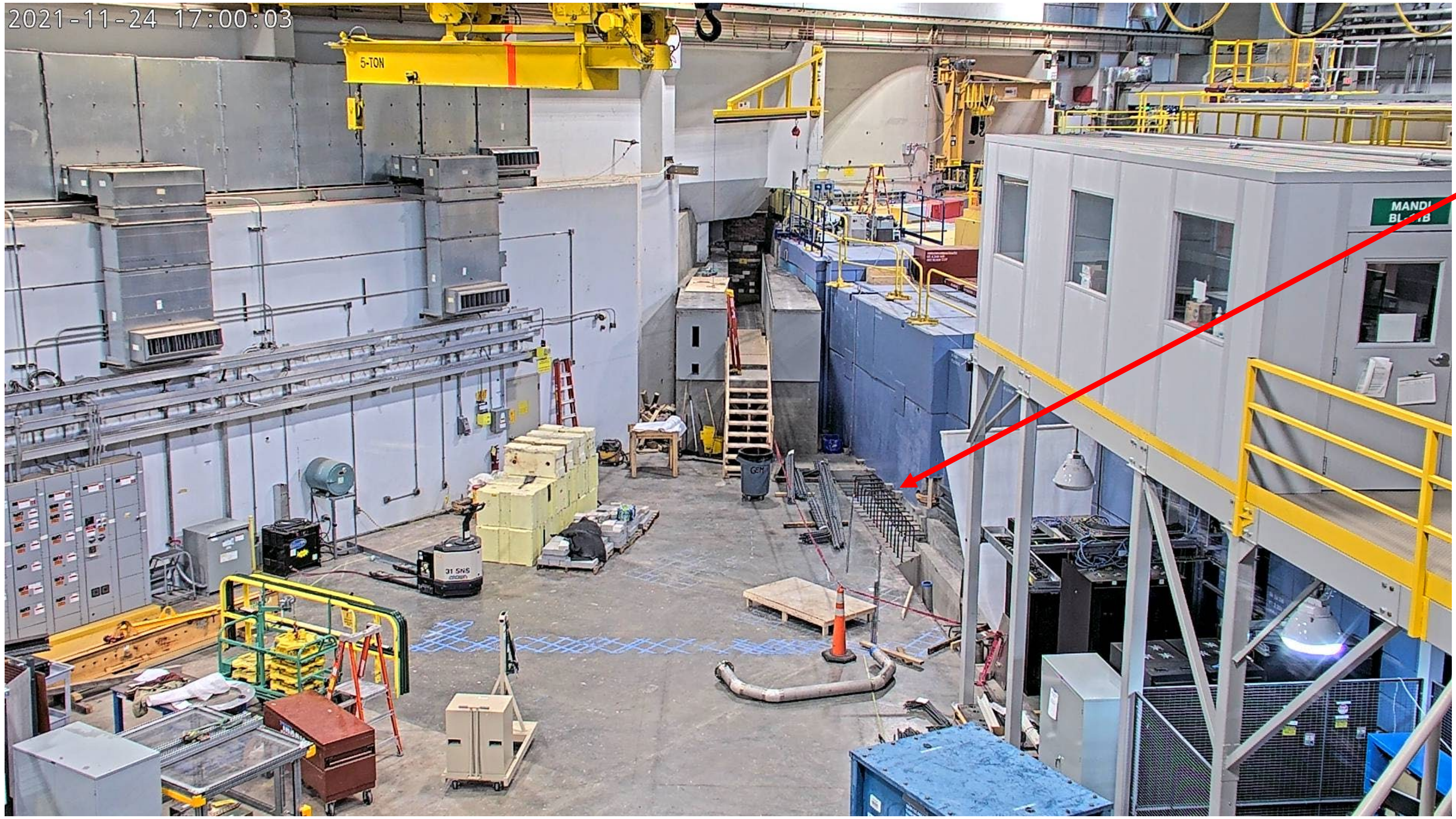
April 2021

October 2021



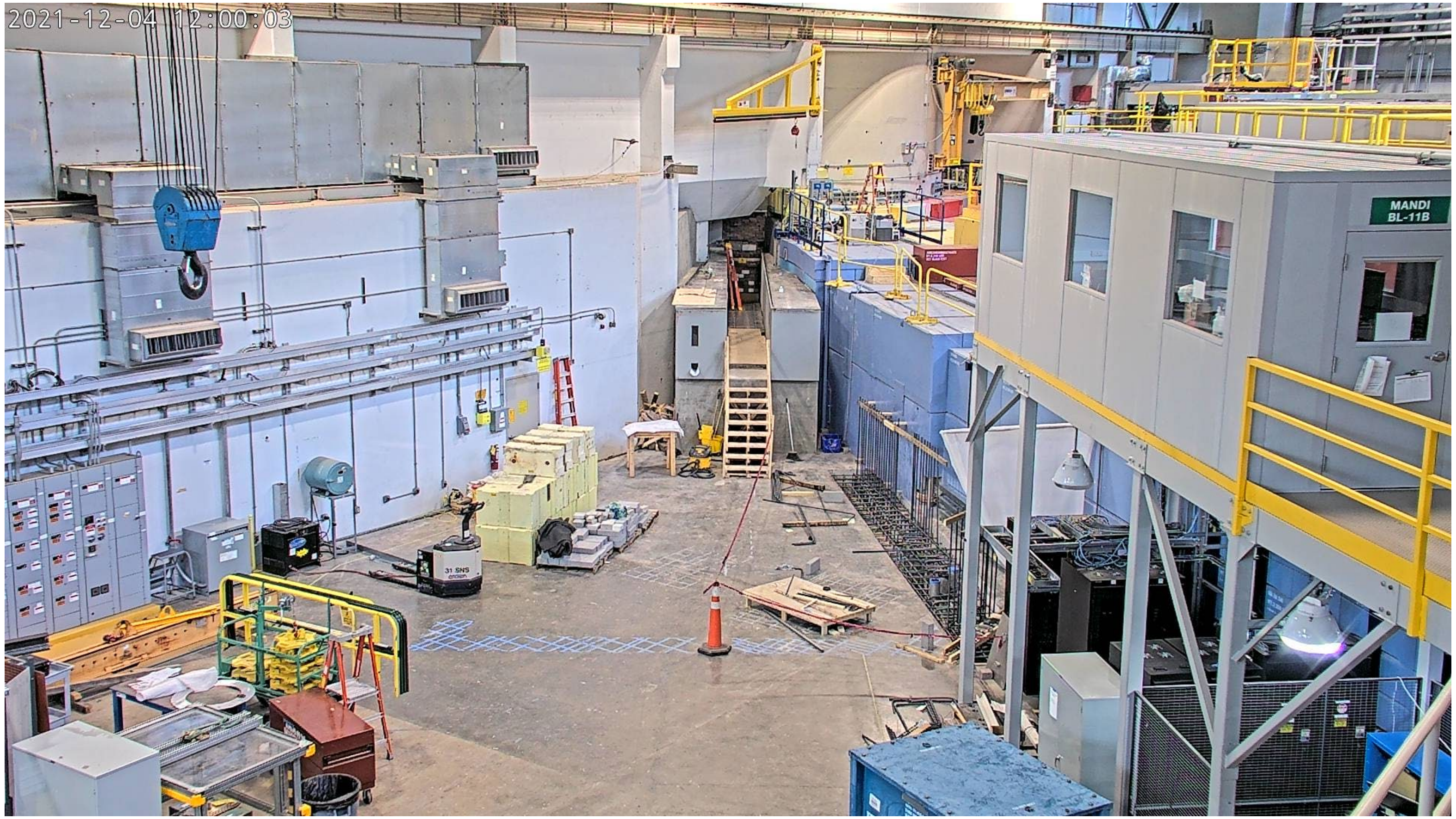
Existing floor rebar is being mapped

November 2021

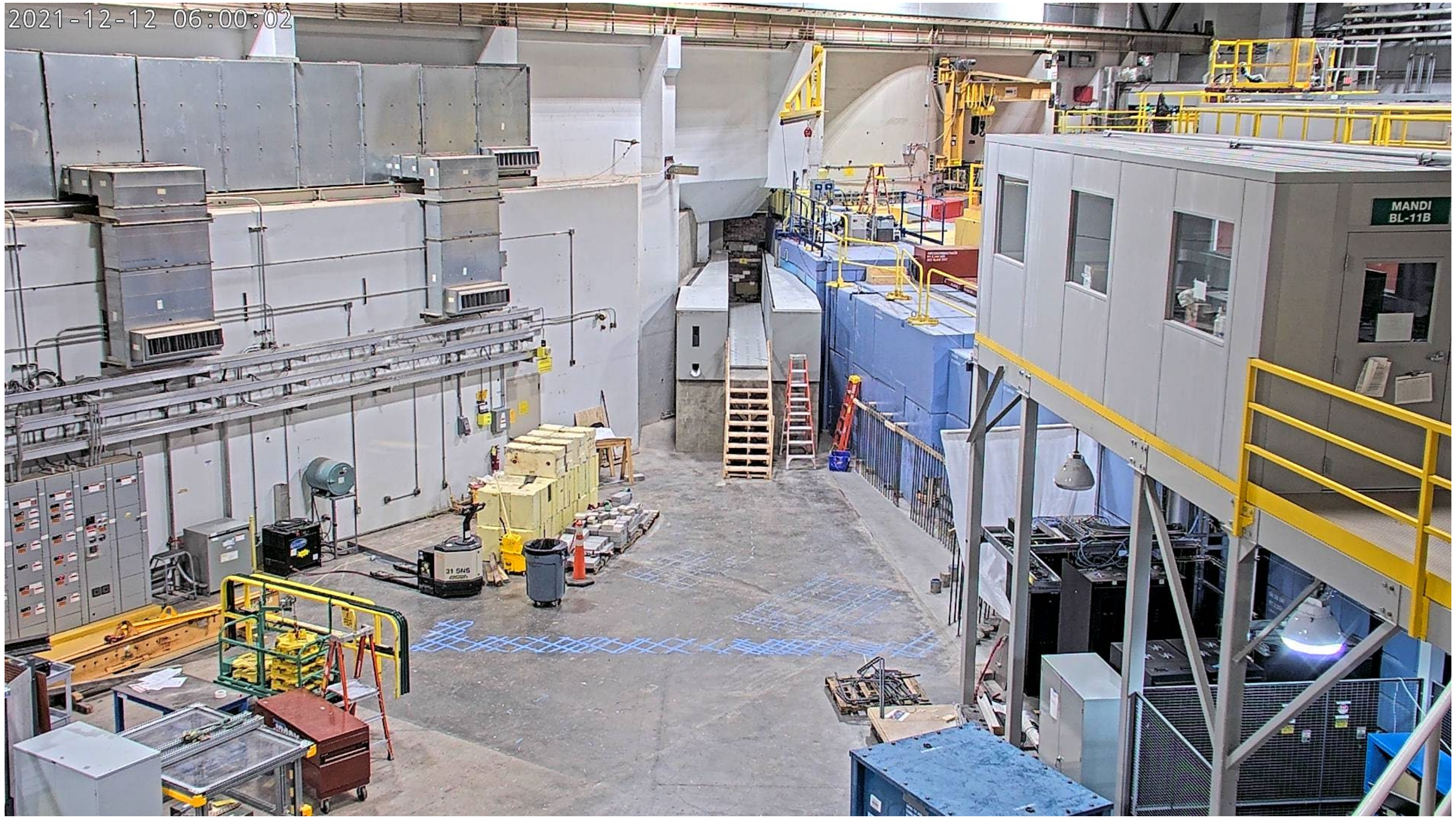


Bi-sector trench filled in preparation to VENUS cave wall

December 2021



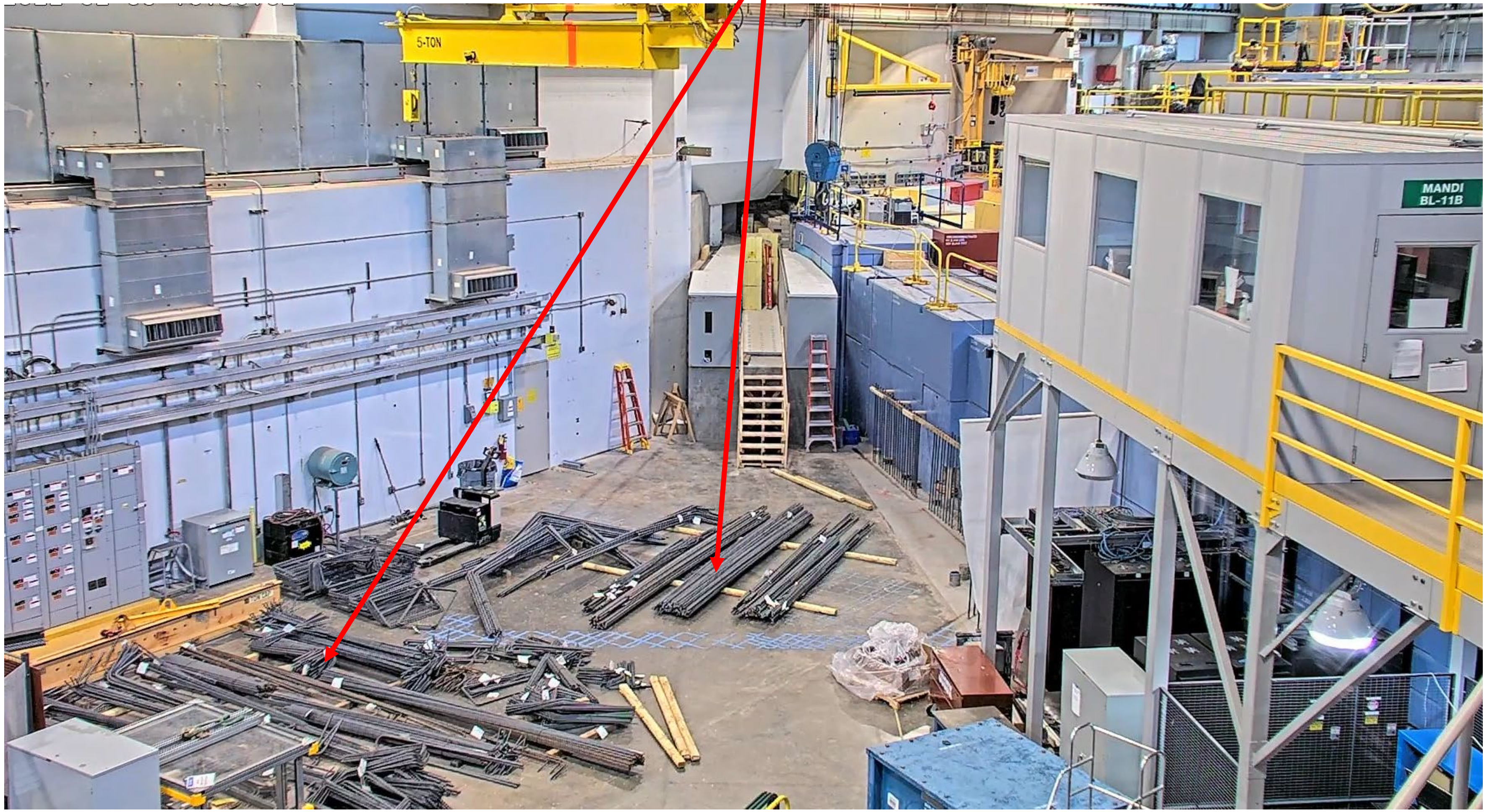
December 2021



January 2022

February 2022

All the beamline rebar has arrived.



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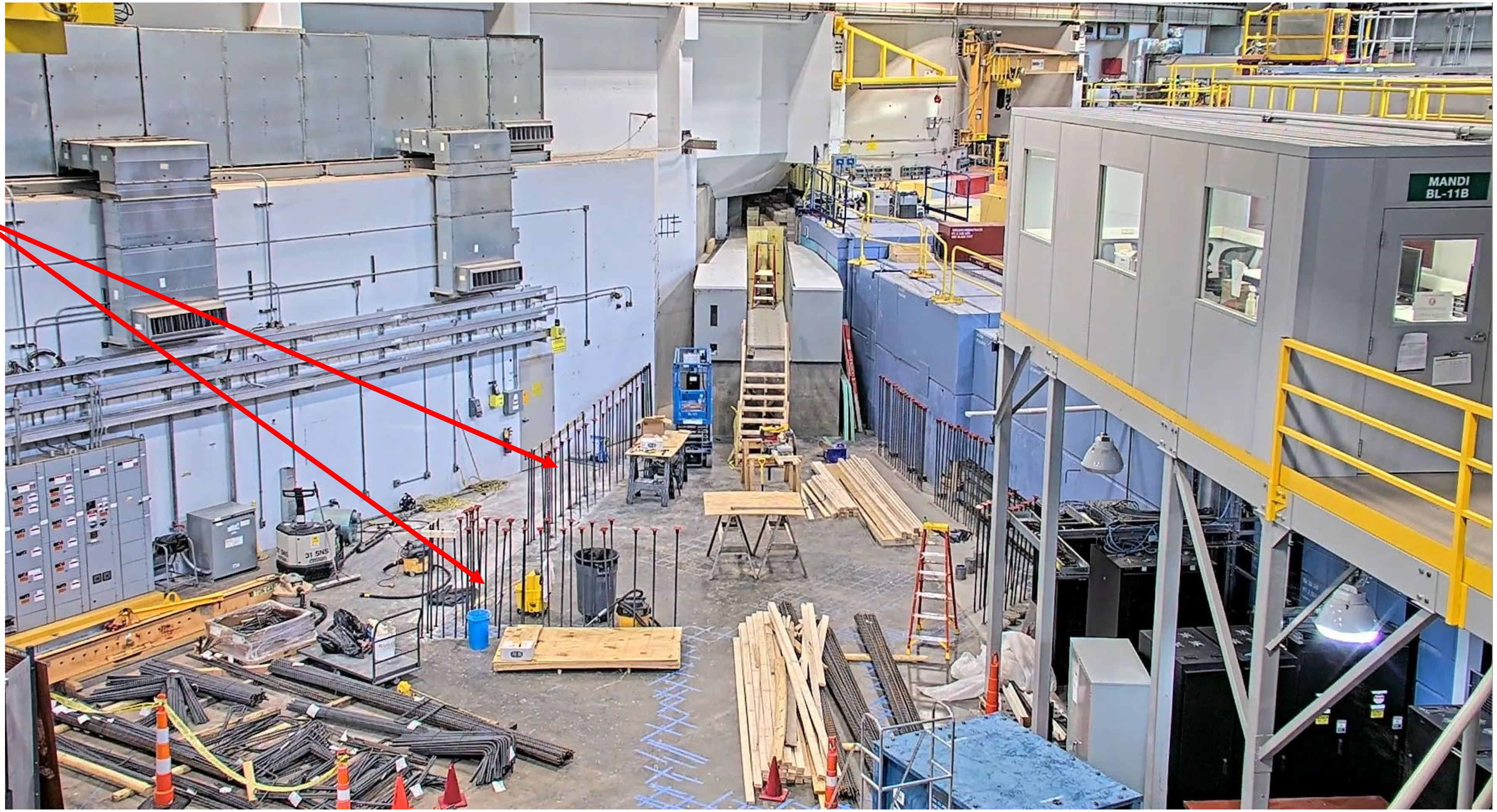
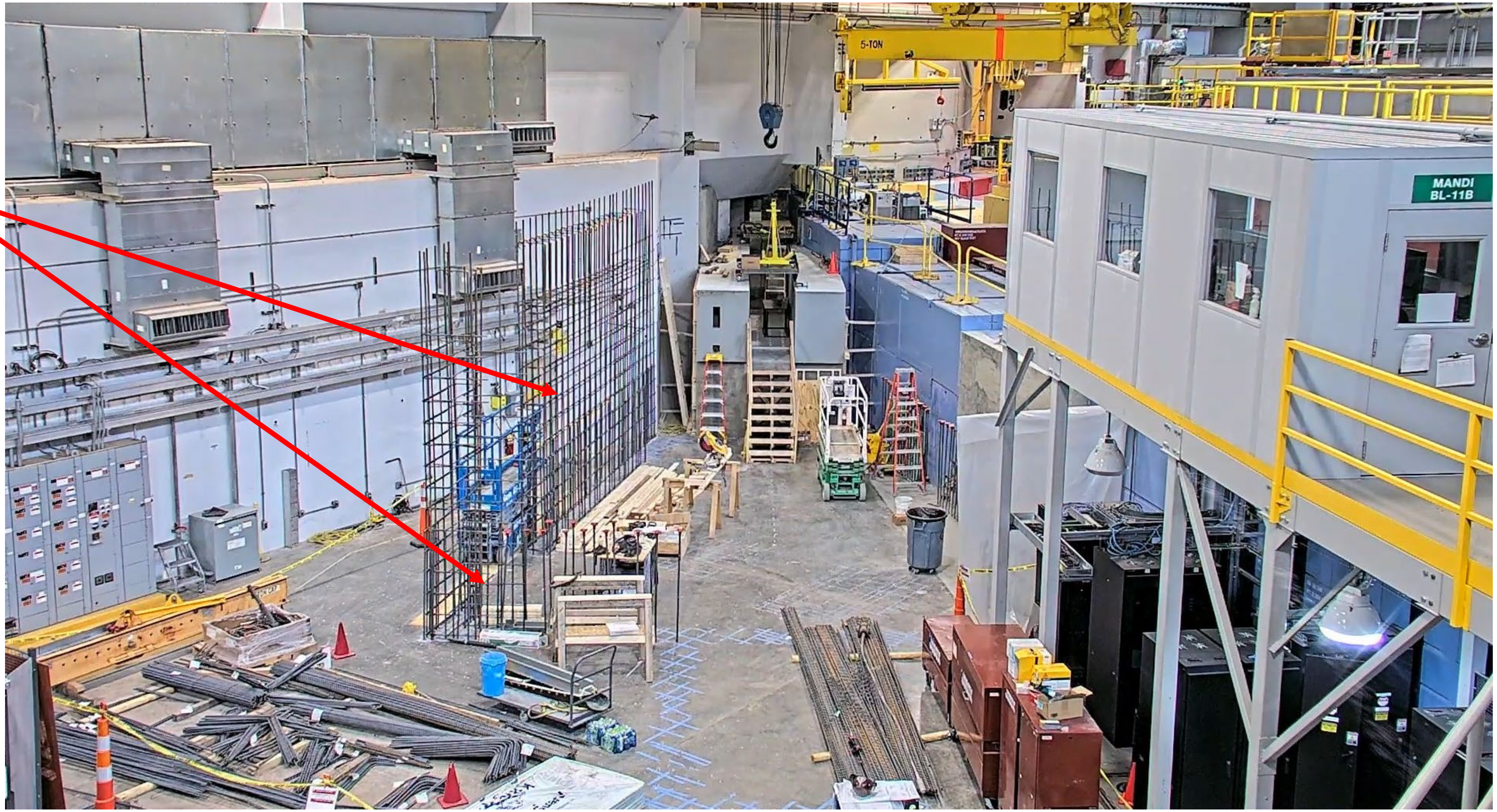
March 2022

VENUS cave wall rebar is installed



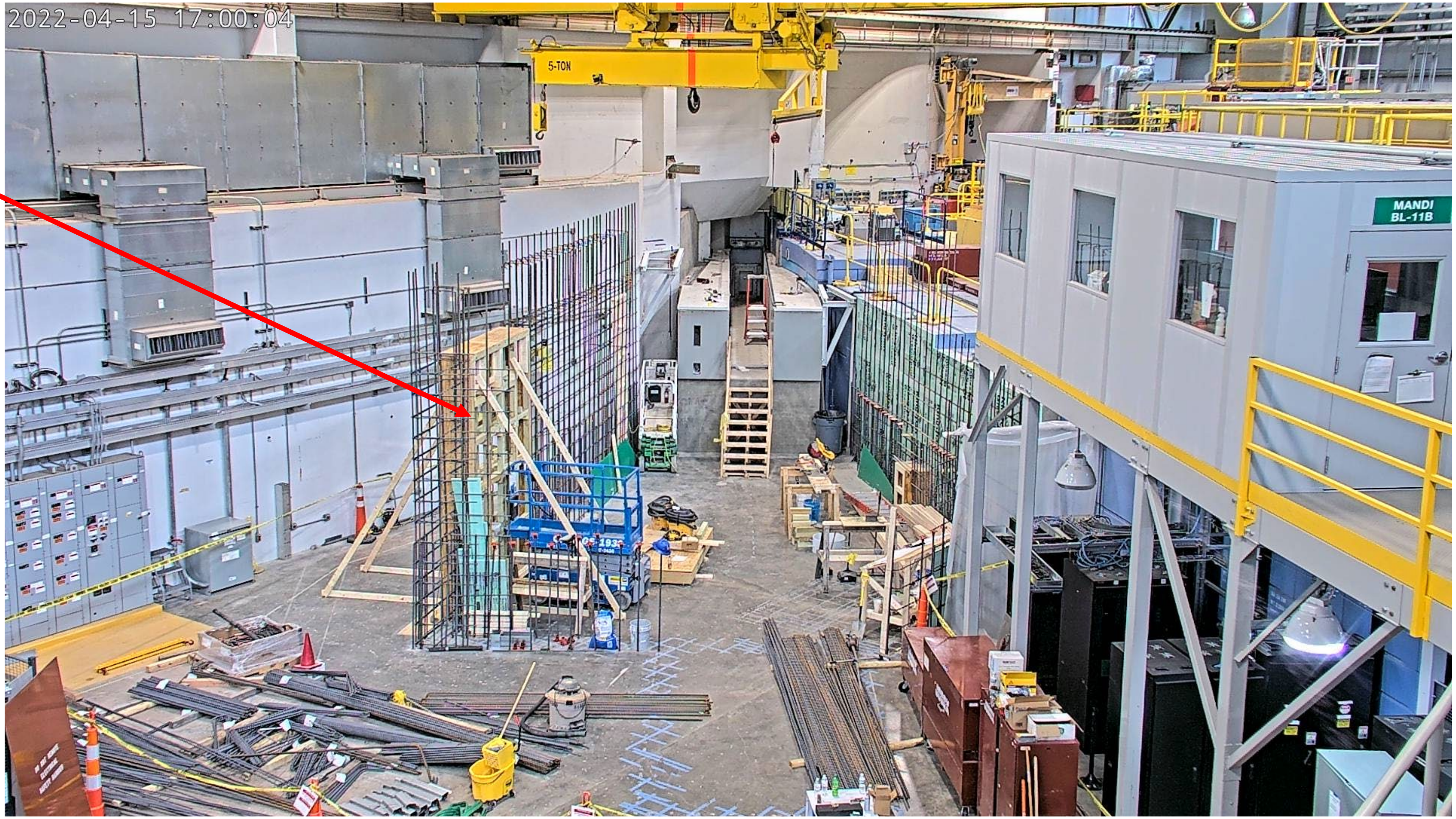
March 2022

VENUS cave wall rebar installation continues



April 2022

Cave door is frame prior to the concrete pour



May 2022

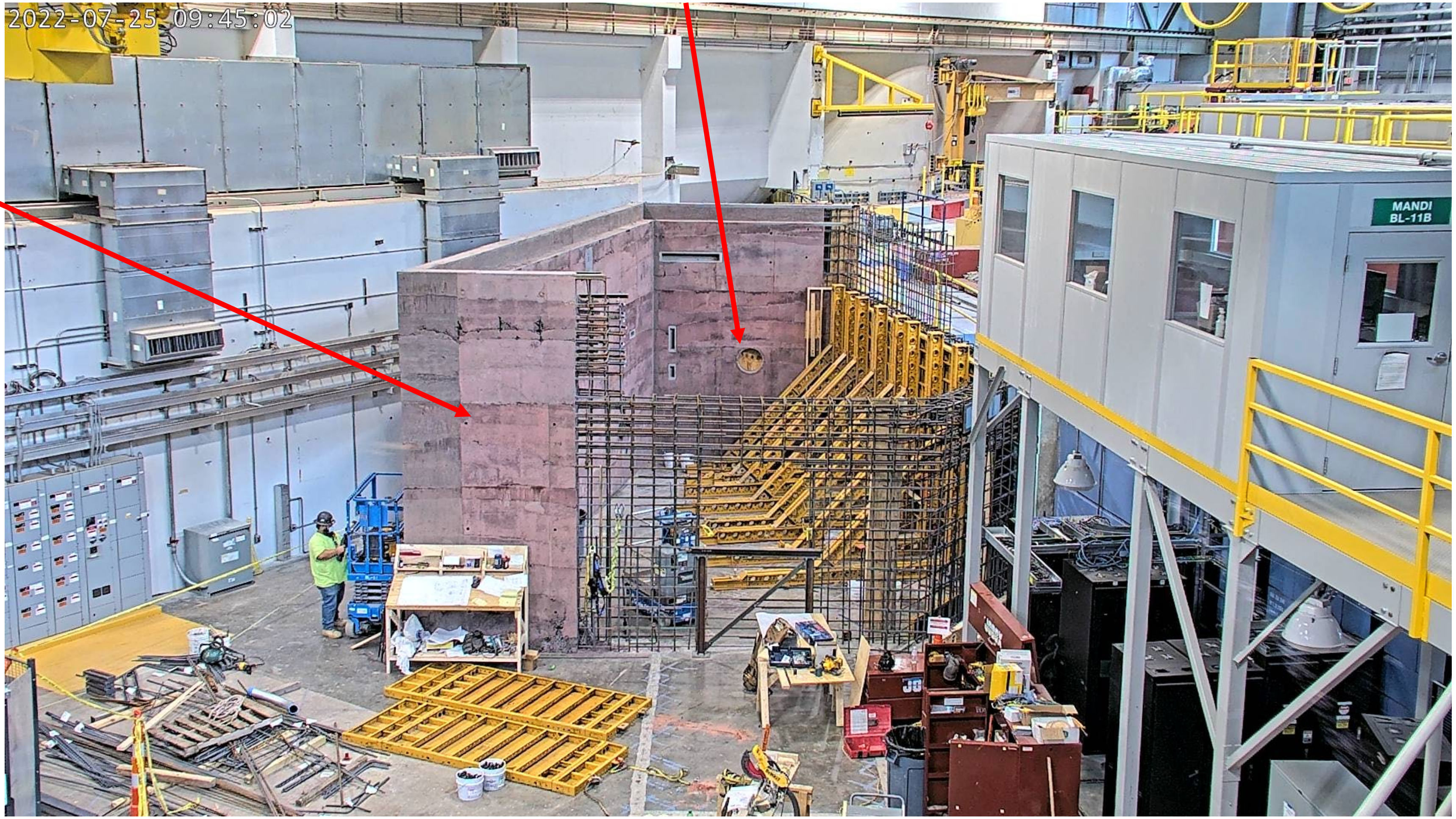
Steel and wood formwork is installed, and HD concrete pour begins

June 2022

July 2022

Opening for neutron beam

Formwork removed giving views of the VENUS cave walls

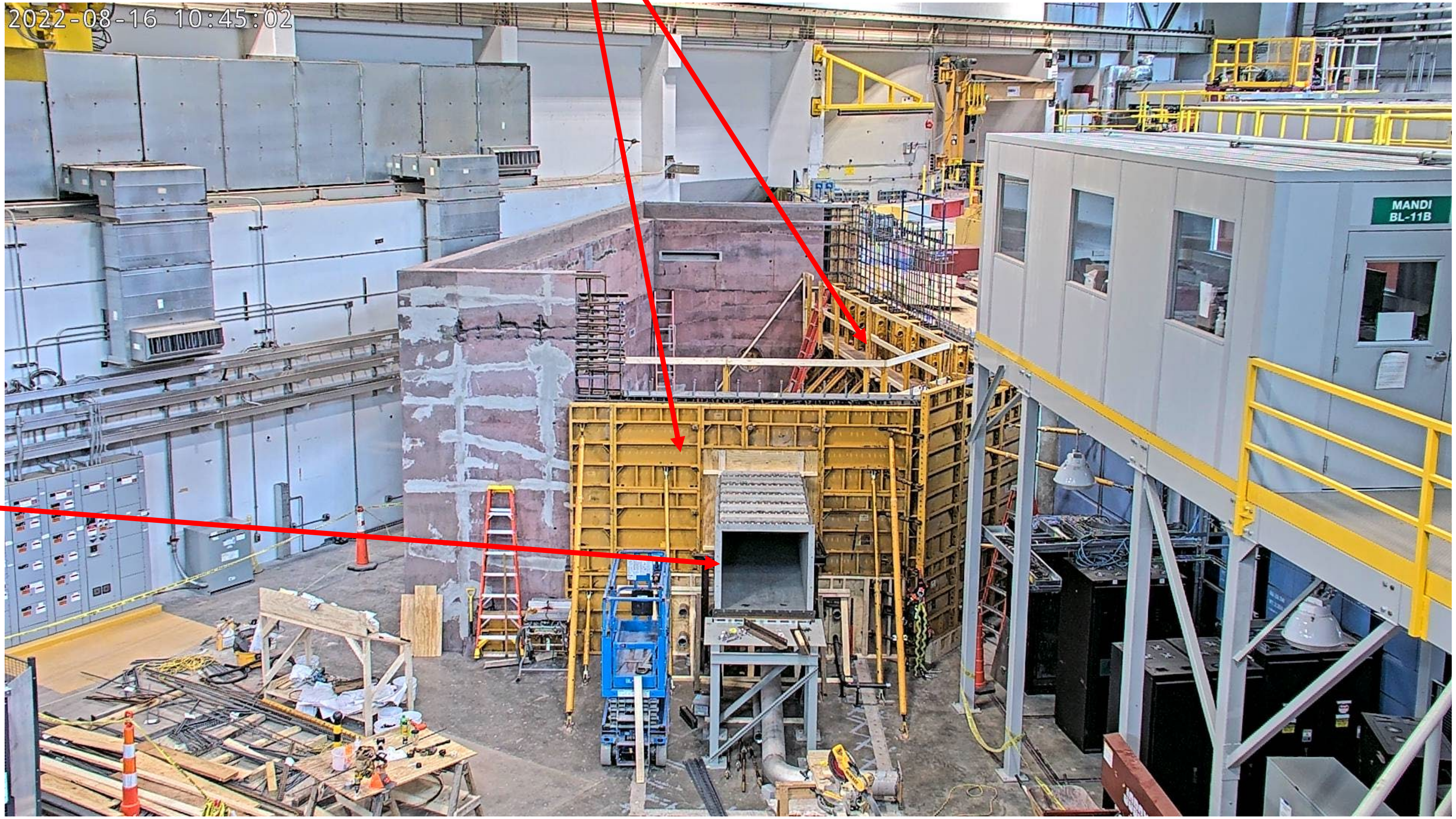


OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

August 2022

Formwork installed on the remaining walls

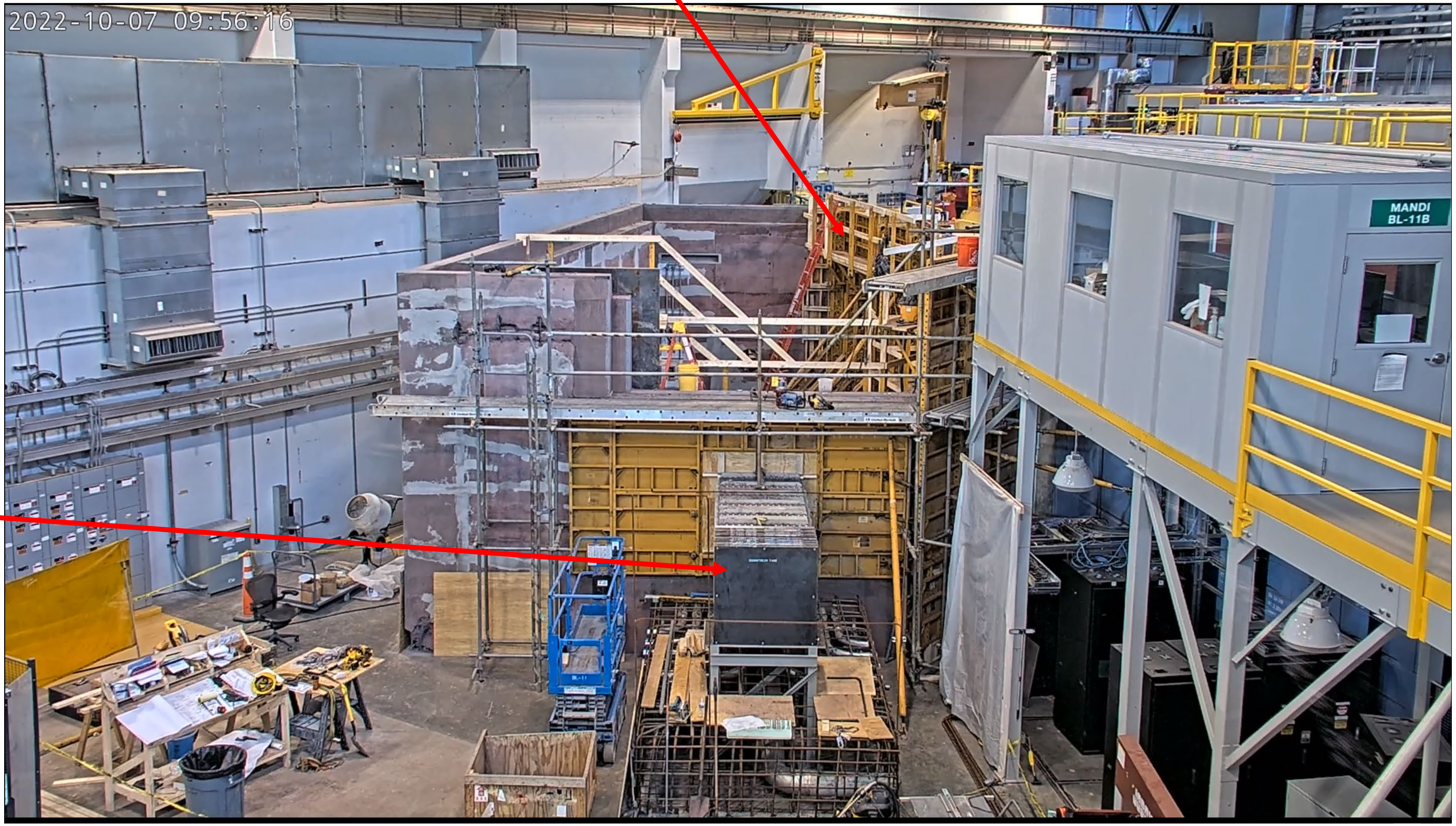
VENUS "get-lost tube" sleeve



October 2022

This side of the VENUS walls is poured

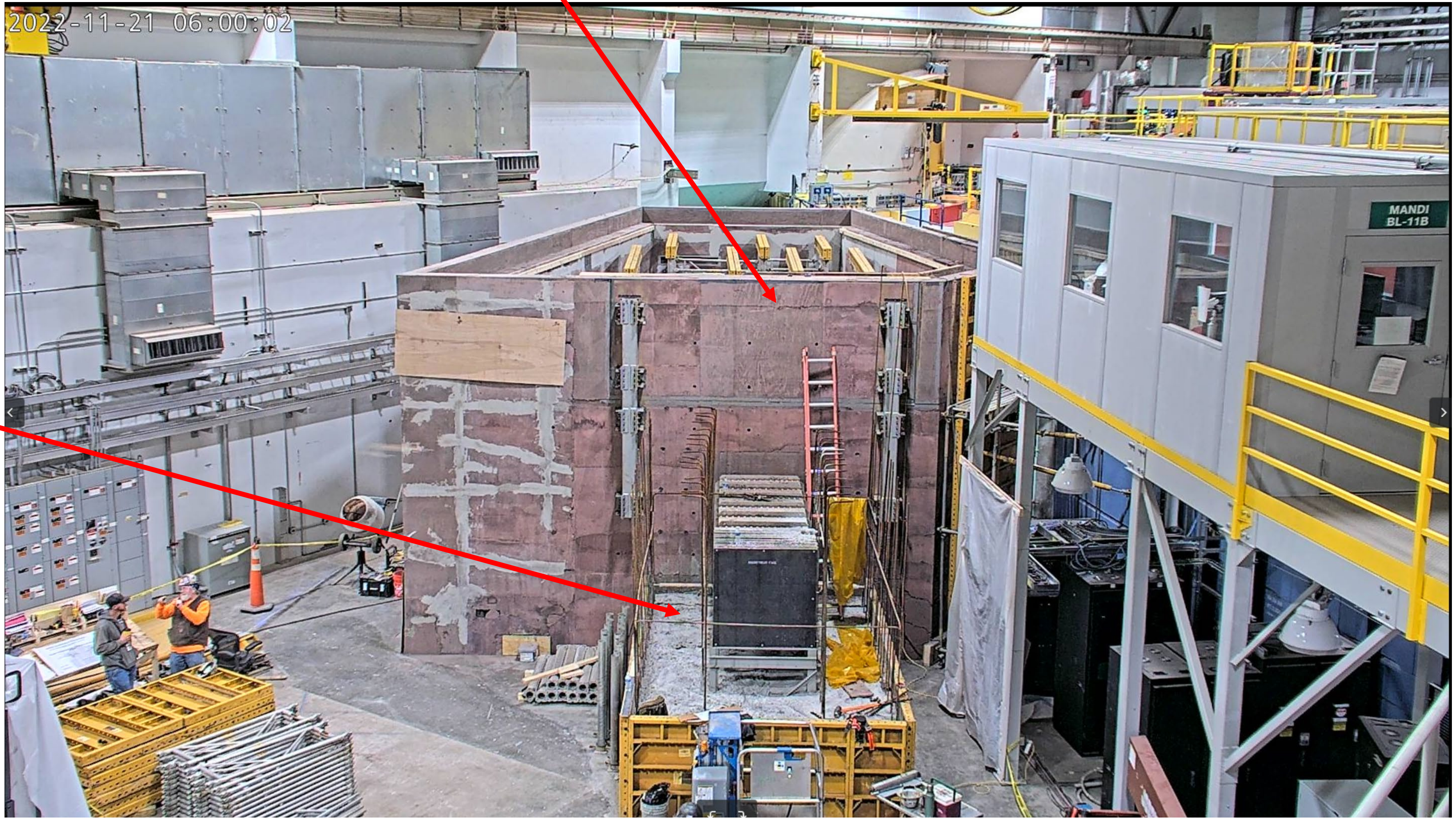
VENUS beam stop installed (made of B_4C, steel and polyethylene)



November 2022

The VENUS cave walls
are all poured

Beam stop
being
poured



December 2022

Prepping for the roof beams

Beam stop completed poured

January 2023

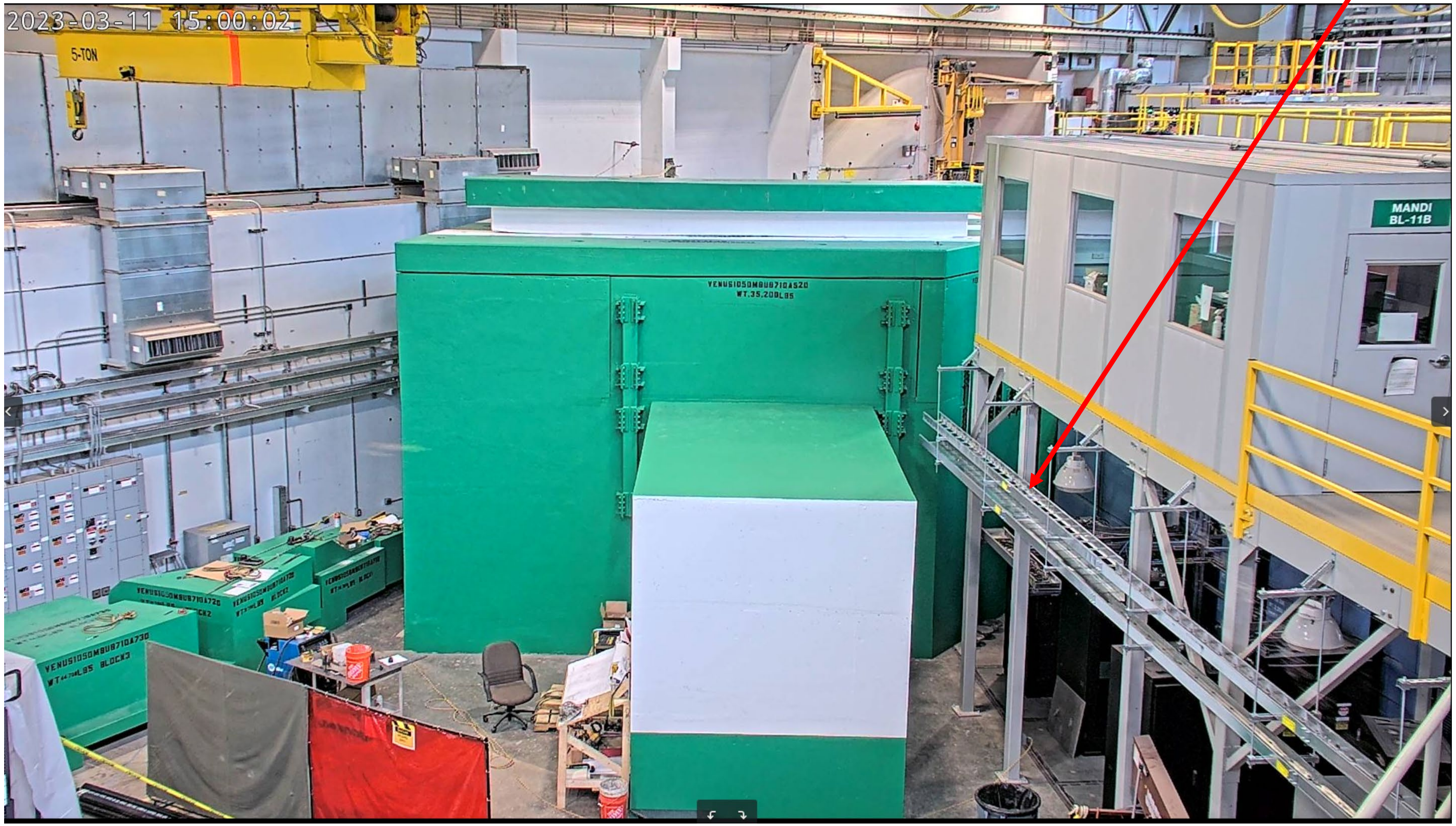
All roof beams are poured

Removed beam stop formwork

February 2023 – Painting VENUS!

March 2023

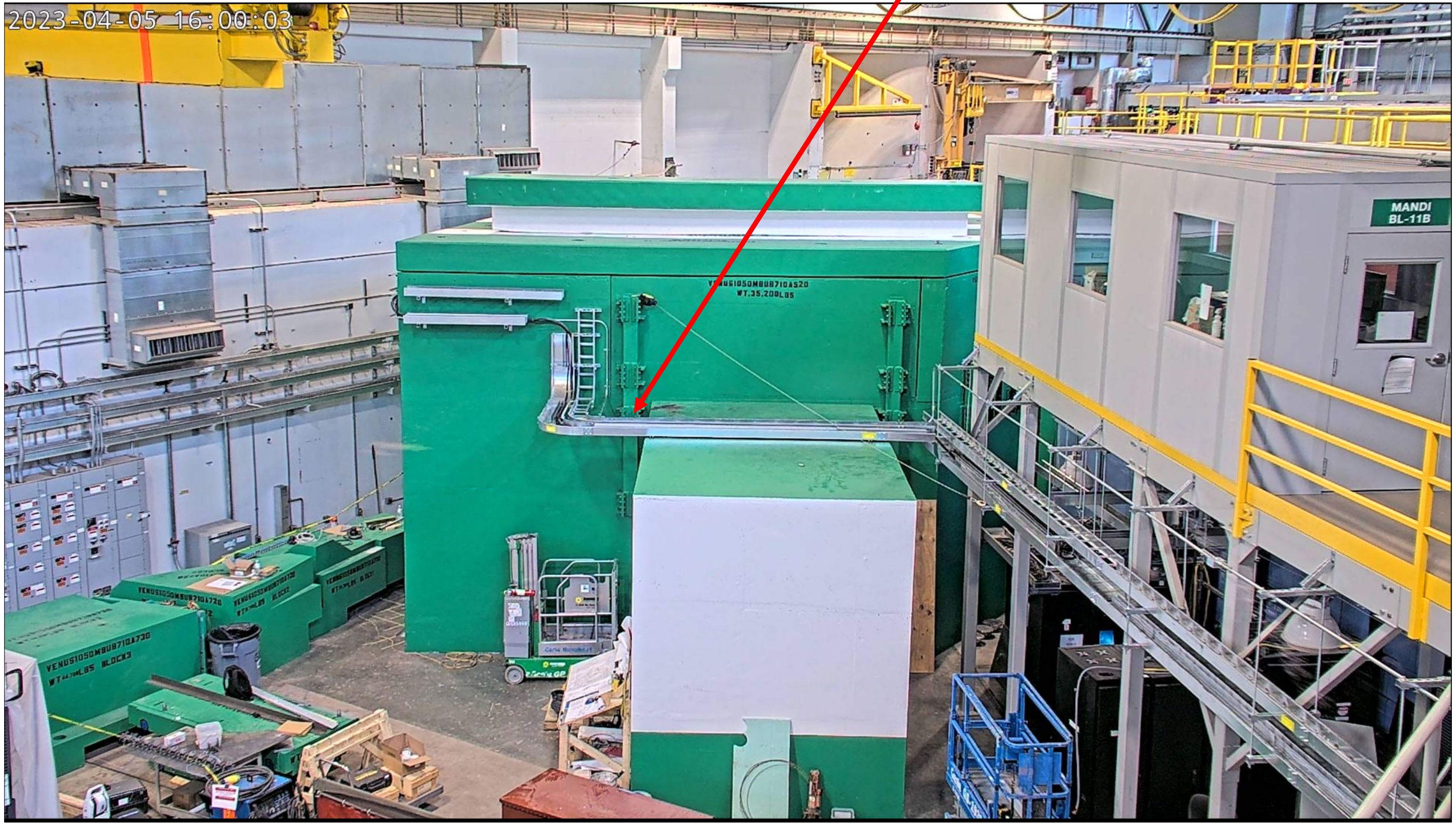
Cable trays are installed



OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

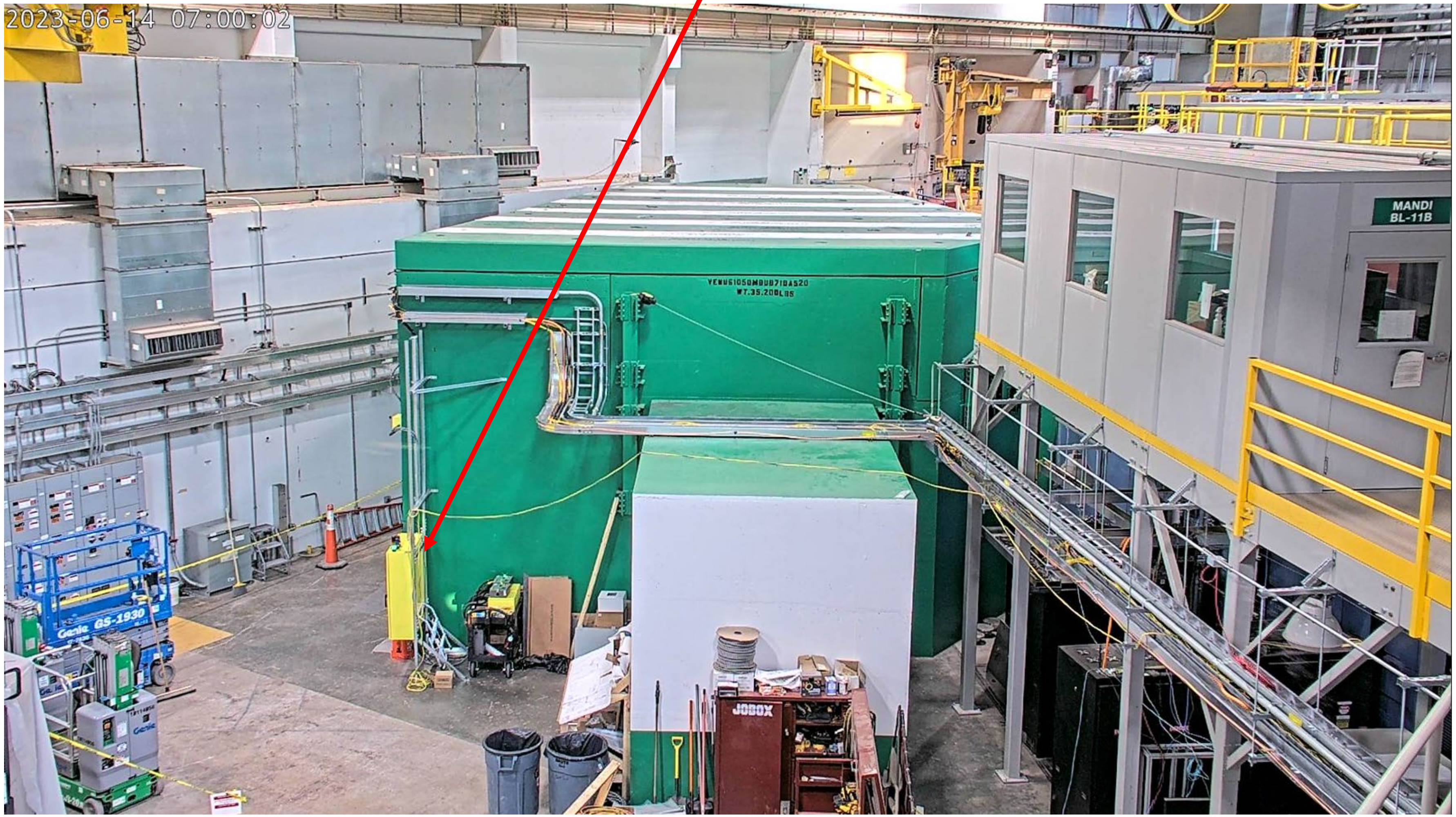
April 2023

Cable trays are installed



June 2023

Shutter controls certified and operational



Side Camera

March 2022

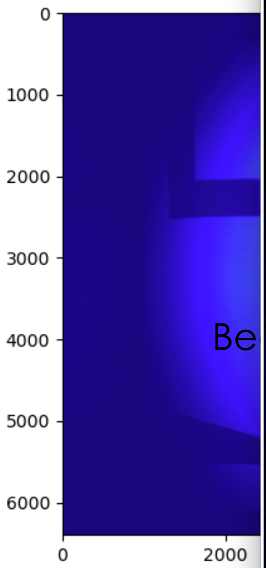
April 2023

May 2023

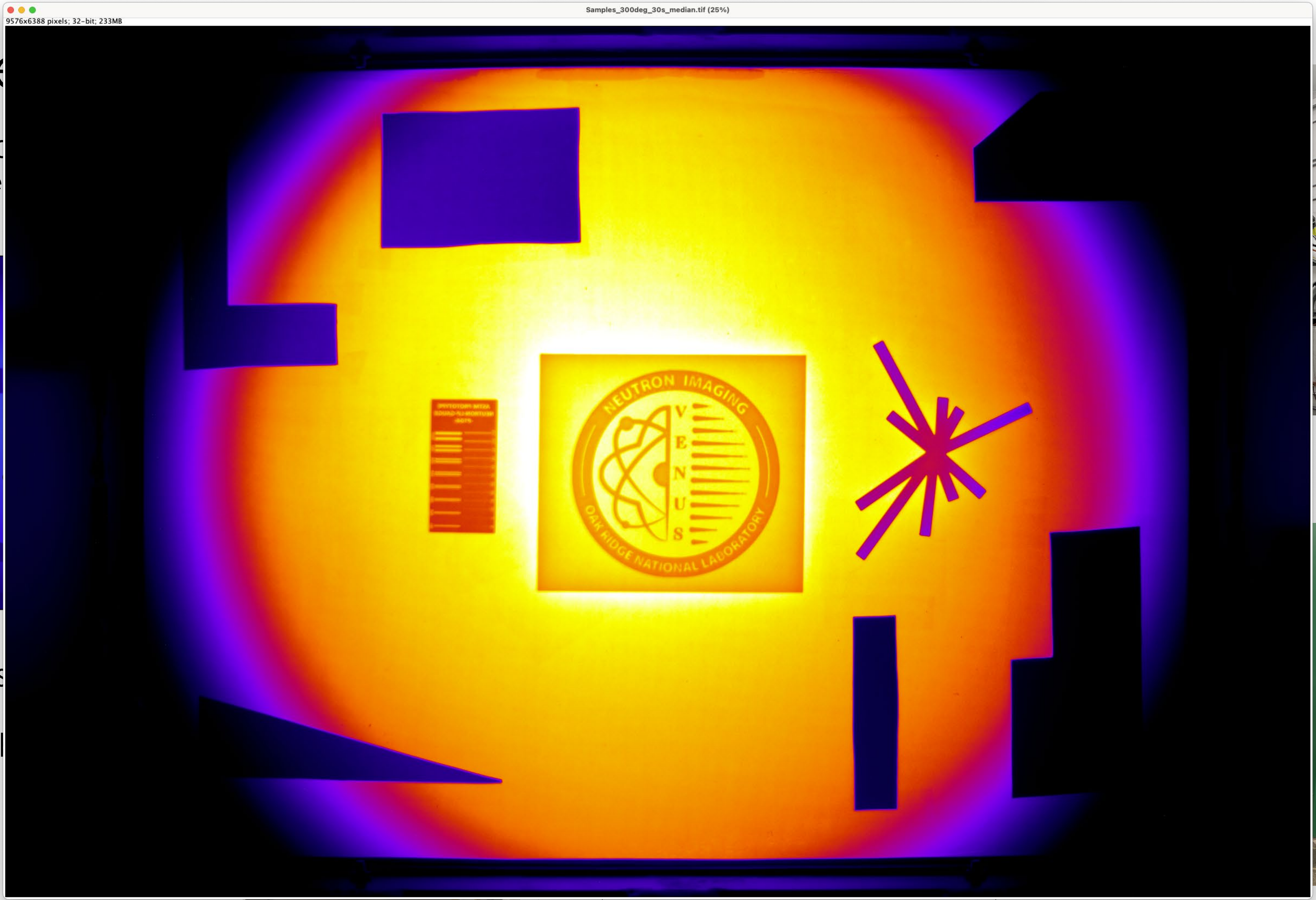
June 2023

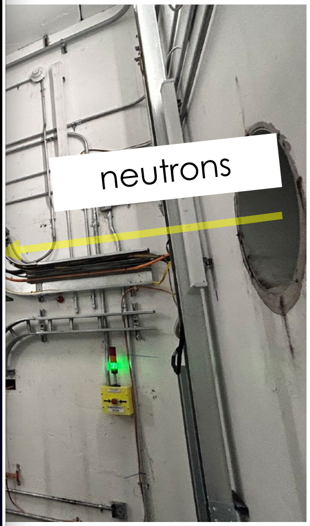
First ne

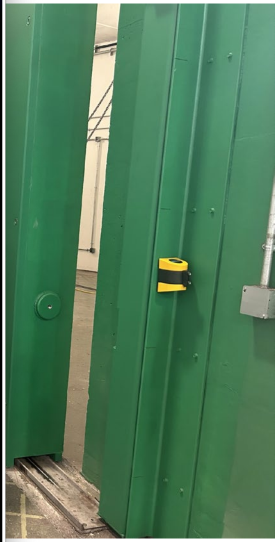
Source po
30 s white

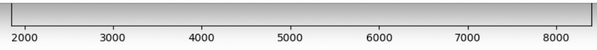


Detector s
- -11
- 16-l









Outline

- Neutron imaging facilities at ORNL
- Principle of time-of-flight (TOF) or hyperspectral neutron imaging
- Resonance imaging
- Bragg edge imaging
- Software efforts
- VENUS
- **Conclusion**

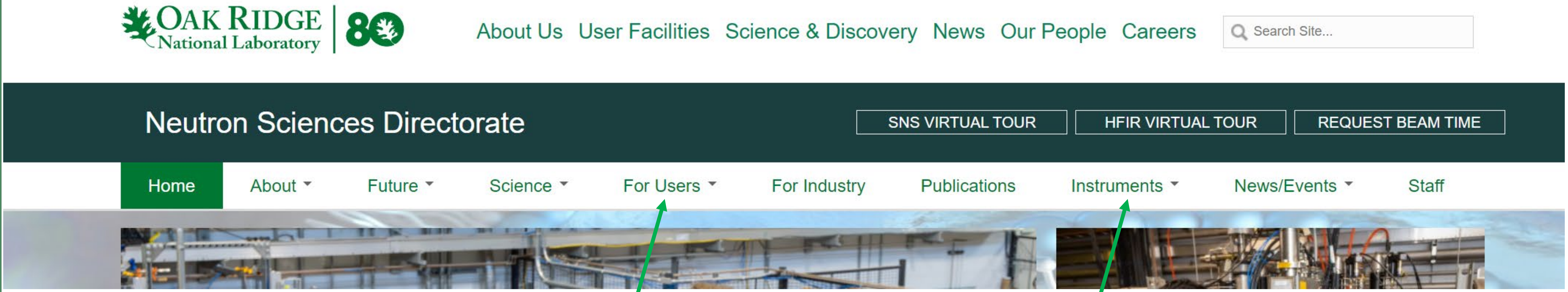
Conclusion

- The VENUS beamline will enter its commissioning phase/hybrid user program in 2024.
- Science at VENUS will benefit from two unique capabilities:
  - Bragg edge imaging
  - Resonance imaging
- These techniques may benefit Earth and planetary materials
- The use of advanced software such as HyperCT and iBeatles will enhance our ability to measure and analyze data
- The future of neutron imaging is bright!

Thank you

The portion of this research used resources at the SNS and HFIR, DOE Office of Science User Facilities operated by the Oak Ridge National Laboratory.

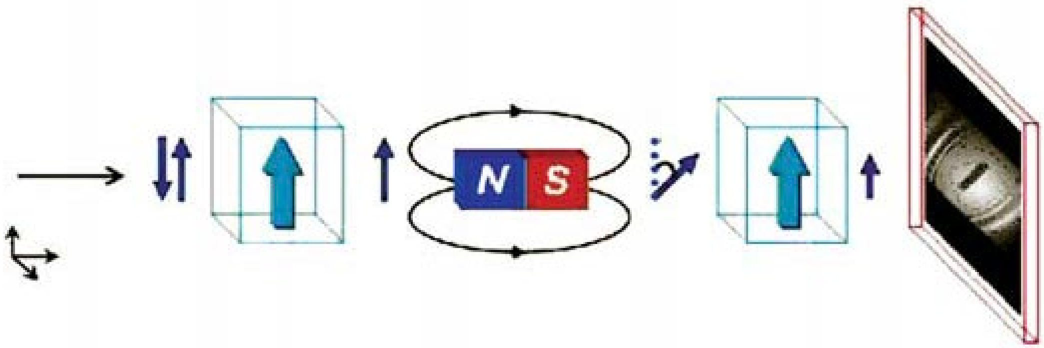
neutrons.ornl.gov



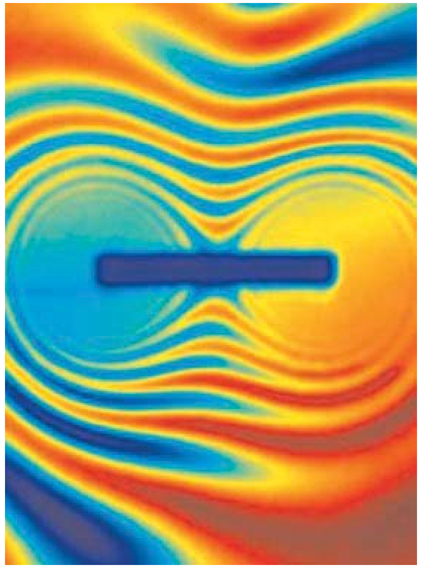
How to collaborate with us

Our beamlines and contact information

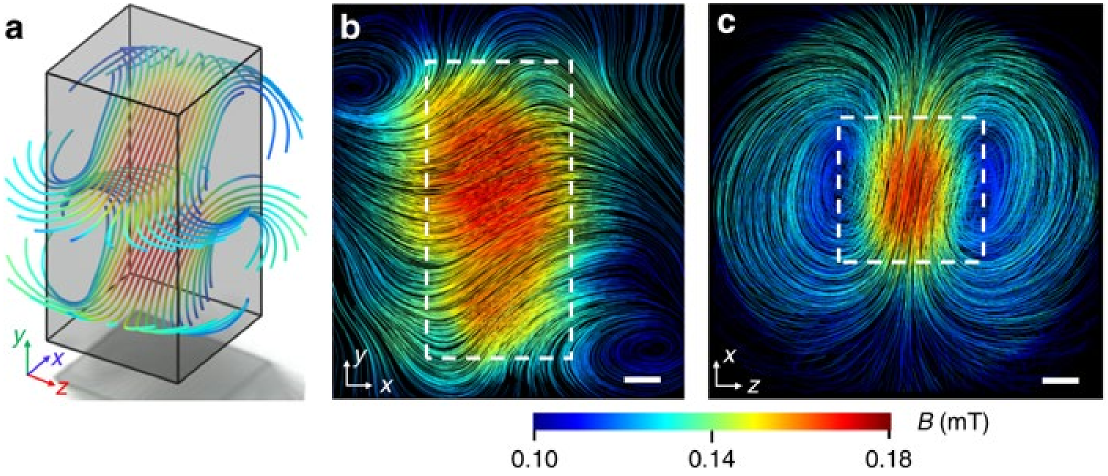
Polarized Neutron Imaging



Kardjilov et al., ADVANCED MATERIALS & PROCESSES/JULY 2008



Tensorial neutron tomography of three-dimensional magnetic vector fields in bulk materials



Hilger *et al.*
Nature Communications 9, 4023 (2018)