SWEDNESS/LINXS Doctoral-level course on neutron imaging

Tuesday, 18 May 2021

Planning and running a neutron imaging experiment

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AGENDA

- ➢ **Basic considerations (‘do the homework’)**
- ➢ **How to write a good beamtime proposal**
- ➢ **‘Beamtime proposal exercise’**

Planning and running a neutron imaging experiment

www.neutron.anl.gov/facilities.html

Major Neutron Sources

America
- High Flux Isotope Reactor (HFIR), Oak Ridge National Laboratory, Tennessee, USA
- Los Alamos Neutron Science Center (LANSCE), New Mexico, USA
- NIST Center for Neutron Research, Gaithersburg, Maryland, USA
- Spallation Neutron Source, Oak Ridge National Laboratory, Tennessee, USA

Asia
- Japan Proton Accelerator Research Complex (J-PARC), Tokai, Japan

Europe
- Budapest Neutron Centre, AEKI, Budapest, Hungary
- Berlin Neutron Scattering Center, Helmholtz-Zentrum, Berlin, Germany
- FRM-II Research Reactor, Garching, Germany
- Institut Laue Langevin, Grenoble, France
- Interfacultair Reactor Instituut, Delft University of Technology, Netherlands
- ISIS Pulsed Neutron and Muon Facility, Rutherford-Appleton Laboratory, Oxfordshire, UK
- Swiss Spallation Neutron Source (SINQ), Villigen Switzerland

Oceania
- Bragg Institute, ANSTO, Australia

- Links for major facilities with extensive user program and Neutron Imaging capabilities

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- Make yourself clear what you want to do and why!
- Check if neutrons are the method of choice (could you use x-rays?)
- Discuss your idea with your supervisor/colleagues -> fine tune
- Check if the experiment is technically feasible
  - ✓ Estimating max allowed sample size (sample attenuation)
  - ✓ Contrast evaluation between the elements (isotopes) you target (cold or thermal neutrons?)

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Some useful references

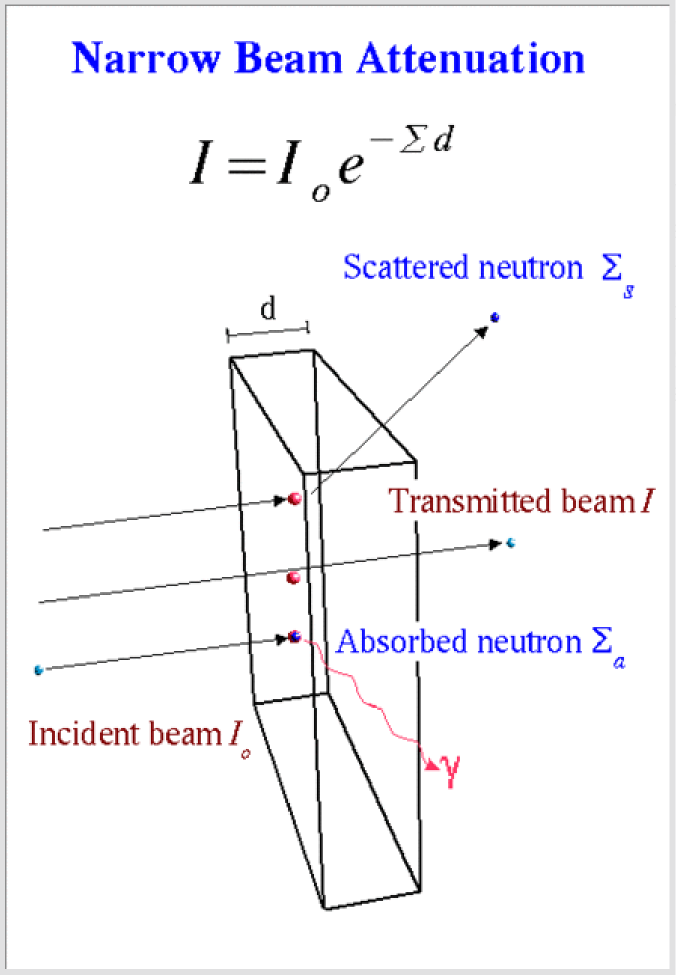

Figure 3: Neutron scattering and capture interaction probabilities.

Image 1 of 3

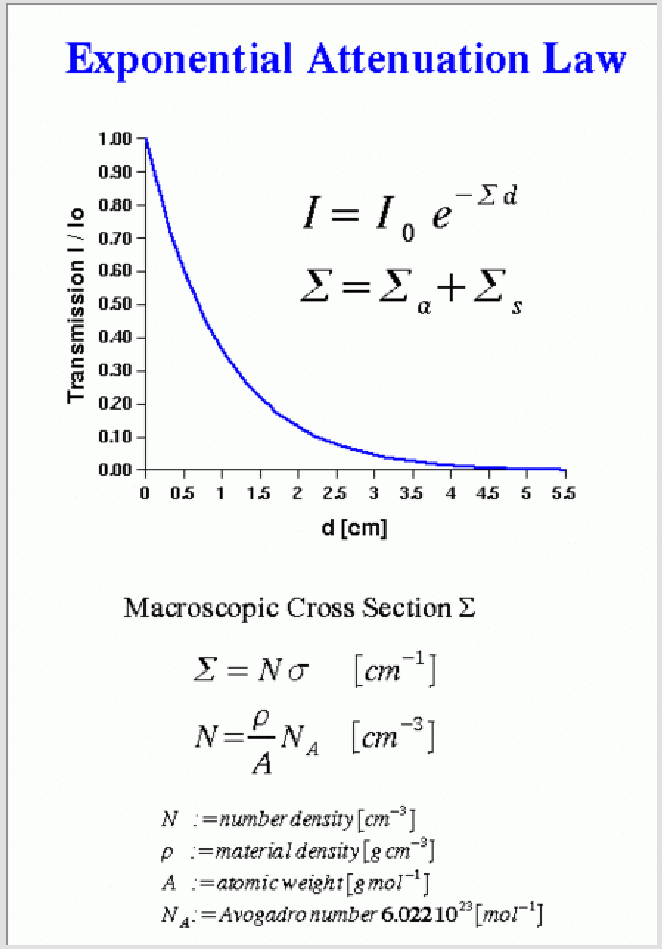

Figure 4: Exponential attenuation of neutrons in matter: Beer-Lambert law.

Image 2 of 3

https://www.psi.ch/niag/neutron-interaction-with-matter

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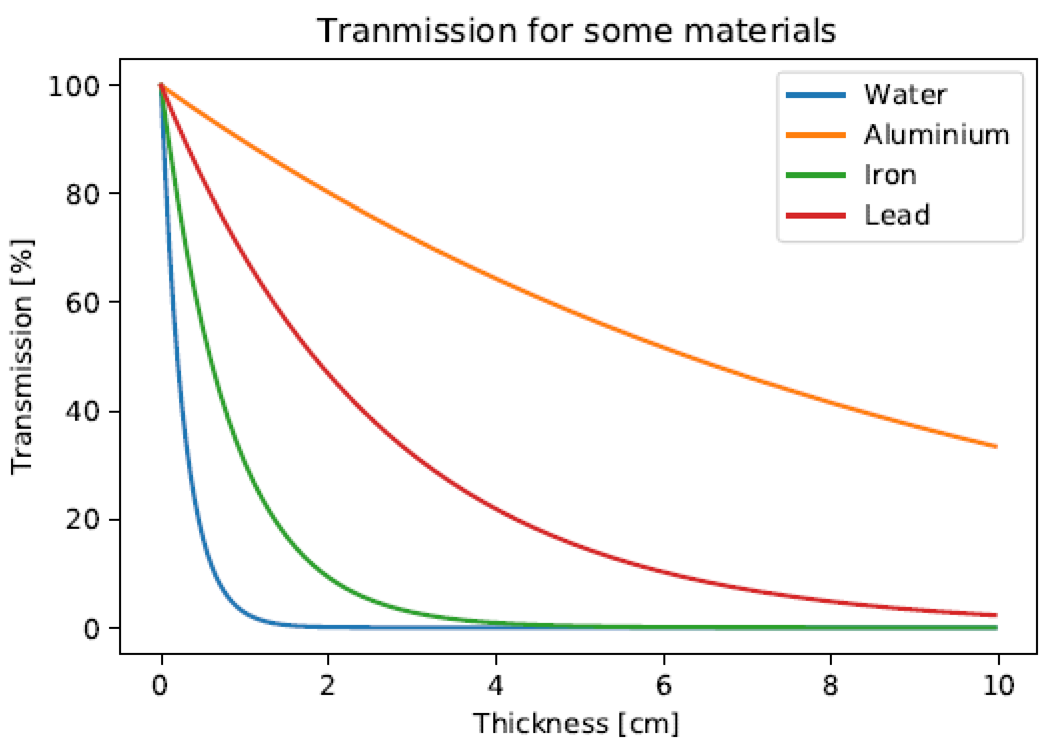
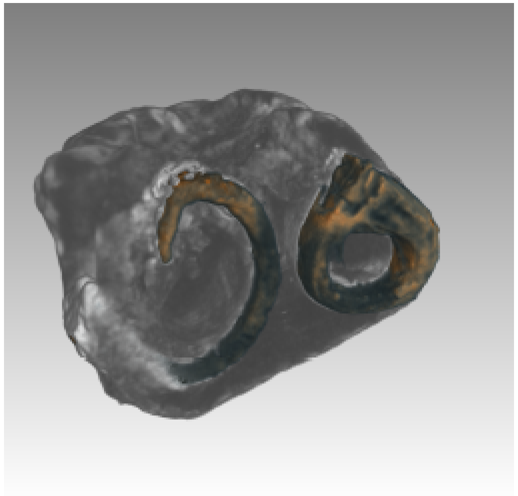
Some useful references

PAUL SCHERRER INSTITUT PSI

Some attenuation examples for neutrons





Neutron tomography of fist-sized lead canon ball from the battle of Bosworth (1485AD)

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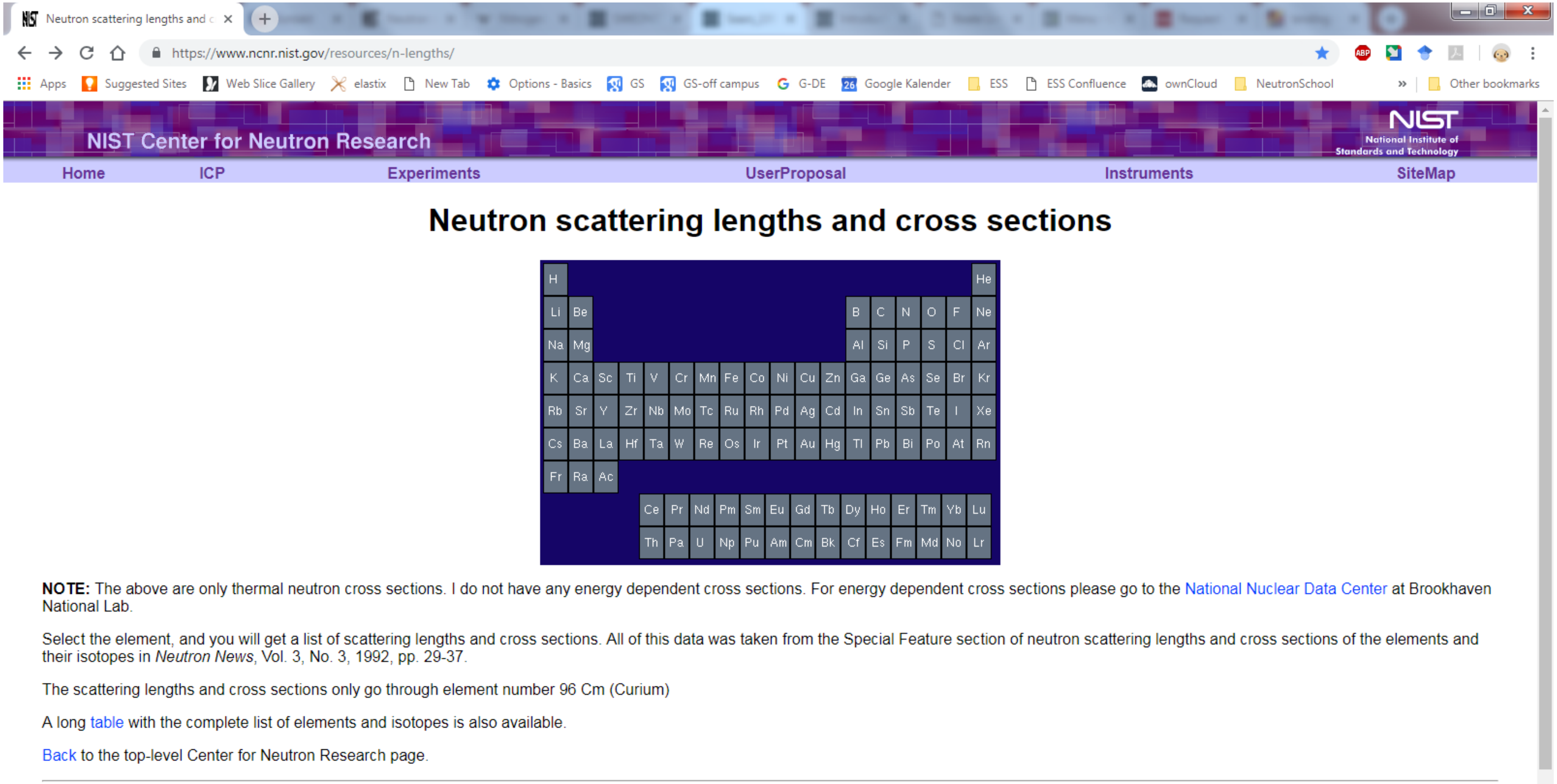
Some useful references

https://www.ncnr.nist.gov/resources/n-lengths/

https://indico.linxs.lu.se/event/62/contributions/428/attachments/12/27/Sears_1992_Neutron_scattering_lengths_and_cross_sections.pdf



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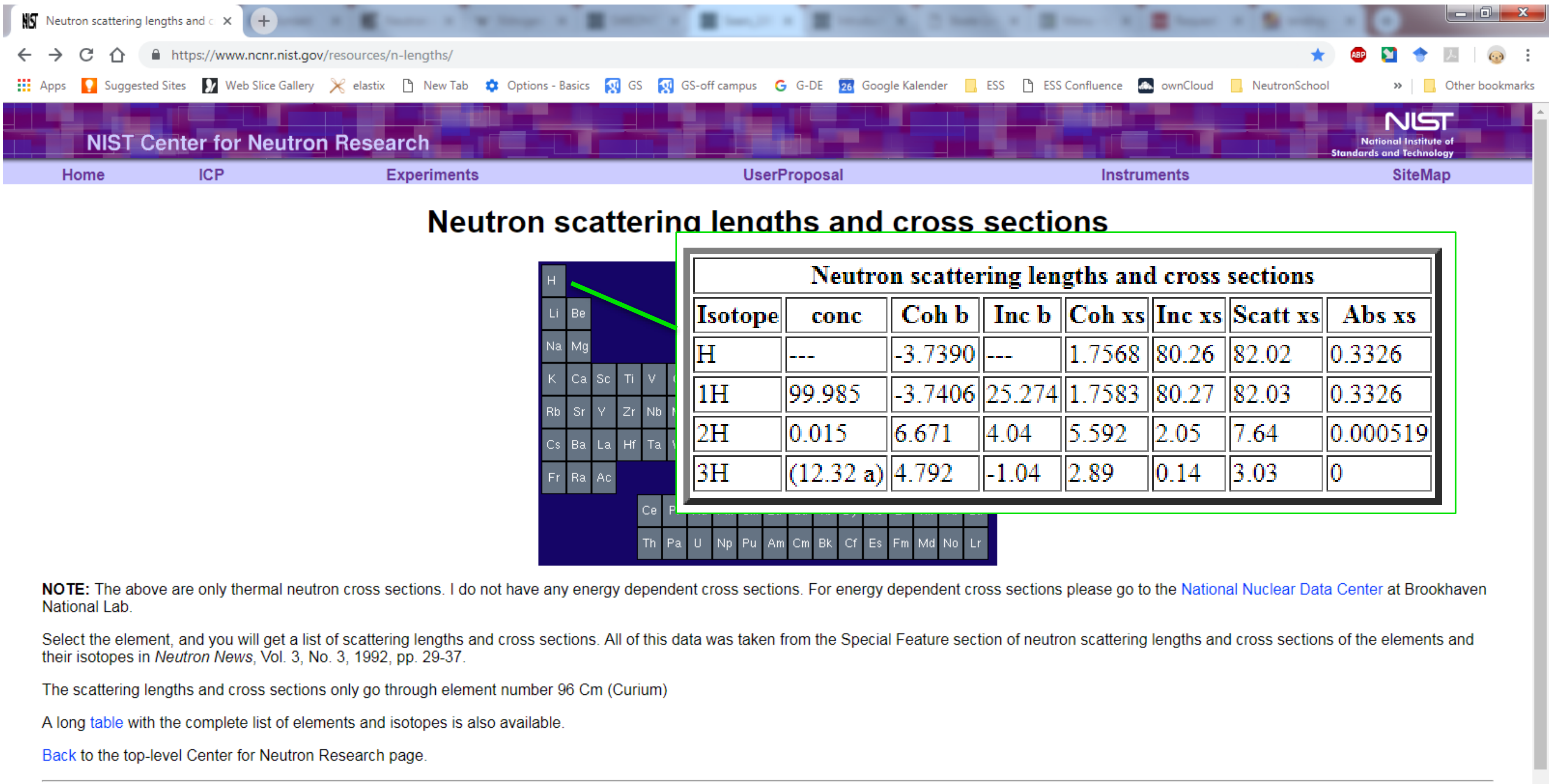


Neutron scattering lengths and cross sections

Neutron scattering lengths and cross sections							
Isotope	conc	Coh b	Inc b	Coh xs	Inc xs	Scatt xs	Abs xs
H	---	-3.7390	---	1.7568	80.26	82.02	0.3326
1H	99.985	-3.7406	25.274	1.7583	80.27	82.03	0.3326
2H	0.015	6.671	4.04	5.592	2.05	7.64	0.000519
3H	(12.32 a)	4.792	-1.04	2.89	0.14	3.03	0

NOTE: The above are only thermal neutron cross sections. I do not have any energy dependent cross sections. For energy dependent cross sections please go to the National Nuclear Data Center at Brookhaven National Lab.

Select the element, and you will get a list of scattering lengths and cross sections. All of this data was taken from the Special Feature section of neutron scattering lengths and cross sections of the elements and their isotopes in *Neutron News*, Vol. 3, No. 3, 1992, pp. 29-37.

The scattering lengths and cross sections only go through element number 96 Cm (Curium)

A long table with the complete list of elements and isotopes is also available.

Back to the top-level Center for Neutron Research page.

Some useful tools for neutron cross sections

Cross-sections calculator 1:
https://www.ncnr.nist.gov/resources/activation

Cross-sections calculator 2:
https://www.ncnr.nist.gov/instruments/bt1/neutron.html

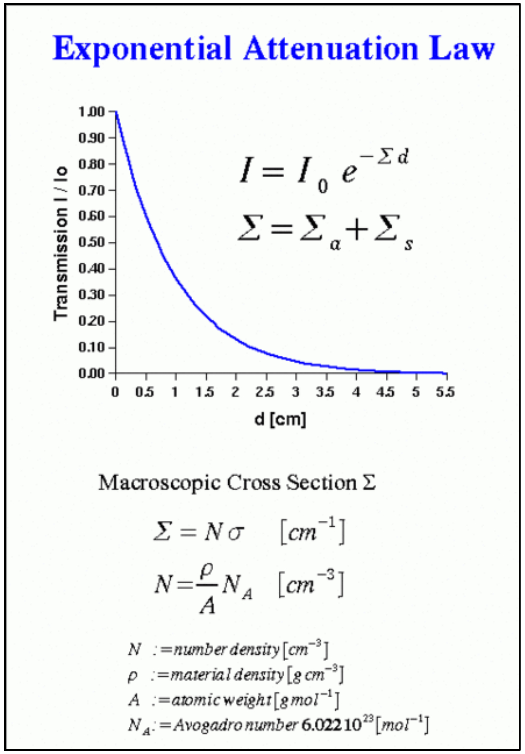
For wavelength dependent cross-sections:
Experimental Nuclear Reaction Data (EXFOR)
https://www-nds.iaea.org/exfor/

Some relevant energies

Wavelength [Å]	Energy [meV]	Energy [eV]	Energy [MeV]
9.04	1	0.001	1.00E-09
4.5	4.03	0.00403	4.03E-09
2.86	10	0.01	1.00E-08
1.8	25	0.025	2.50E-08
0.9	100	0.1	1.00E-07

For wavelength dependent cross-sections:
https://www.oecd-nea.org/janis/book/

For polycrystals (Bragg scattering): -> use nxs_plotter



Planning and running a neutron imaging experiment

- Make yourself clear what you want to do and why!
- Check if neutrons are the method of choice (could you use x-rays?)
- Discuss your idea with your supervisor/colleagues -> fine tune
- Check if the experiment is technically feasible
  - ✓ Estimating max allowed sample size (sample attenuation)
  - ✓ Contrast evaluation between the elements (isotopes) you target (cold or thermal neutrons?)
  - ✓ Decide if radiography (time series?) or tomography
  - ✓ Wavelength resolution needed? Should it be ToF maybe?

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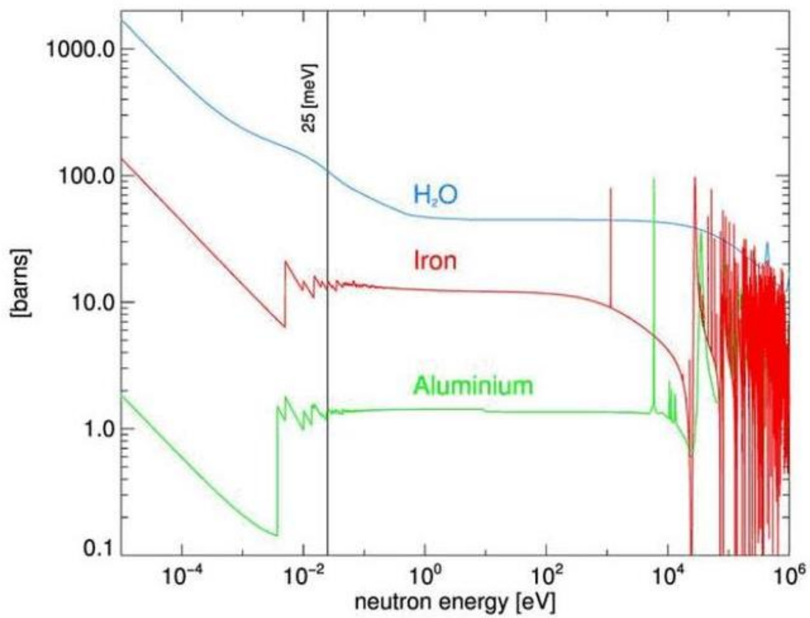
- The wavelength dependent attenuation coefficient (choose the best spectrum for your sample, cold-thermal?, should it be monochromatic?, wavelength selective?)



Thermal neutron cross section at 0.025 eV			
Material	ρ	σ [barns]	Σ [1/cm]
Water	1	112	3.74
Iron	7.9	14	1.18
Aluminium	2.7	1.7	0.1

Figure 5: Energy dependence of neutron cross sections shown for aluminium, iron and the water molecule

Image 3 of 3

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Some useful references

- nxs plotter: calculate the wavelength depended cross sections of polycrystalline materials

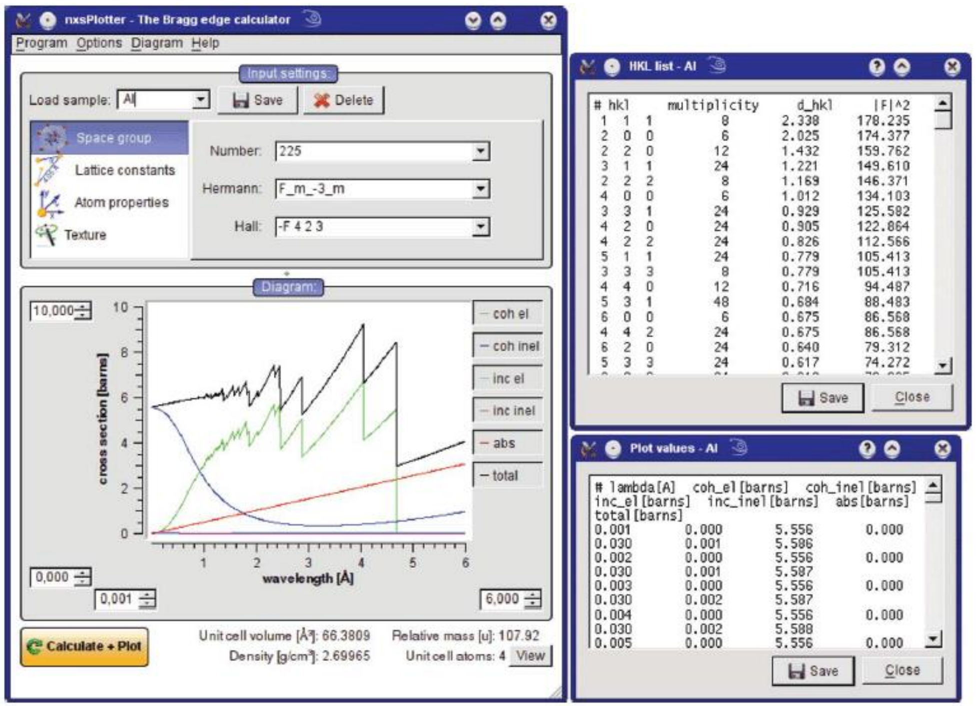
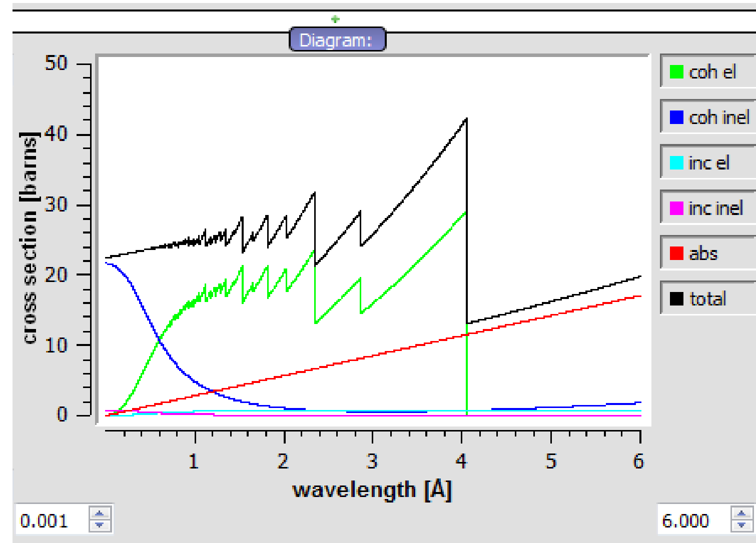
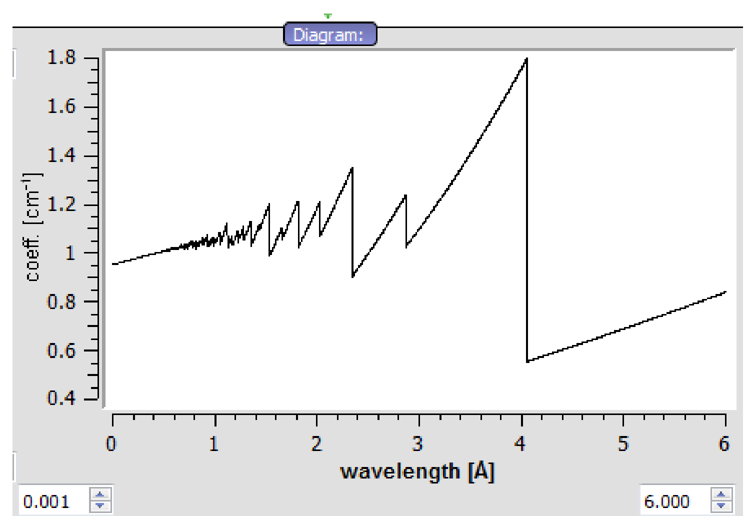


Figure 1

Screenshots of the *nxsPlotter* program, providing a graphical user interface for the *nxs* library routines. (Left) Main GUI showing the cross section spectrum of an aluminium sample. (Right) Tabulated computation results of multiplicities, lattice spacings and structure factors squared for the (*hkl*) lattice planes and neutron cross section values.

https://www.helmholtz-berlin.de/people/boin/nxs_en.html





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- Check if the experiment is technically feasible
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  - ✓ Decide if radiography (time series?) or tomography
  - ✓ Wavelength resolution needed? Should it be ToF maybe?
  - ✓ Would it be relevant to consider using bimodal imaging?
  - ✓ Required resolution to see the features in the images (L/D may play a role)
- Write a a good proposal and convince the reviewers!
- Think about activation of your sample (do you need it back? When?)

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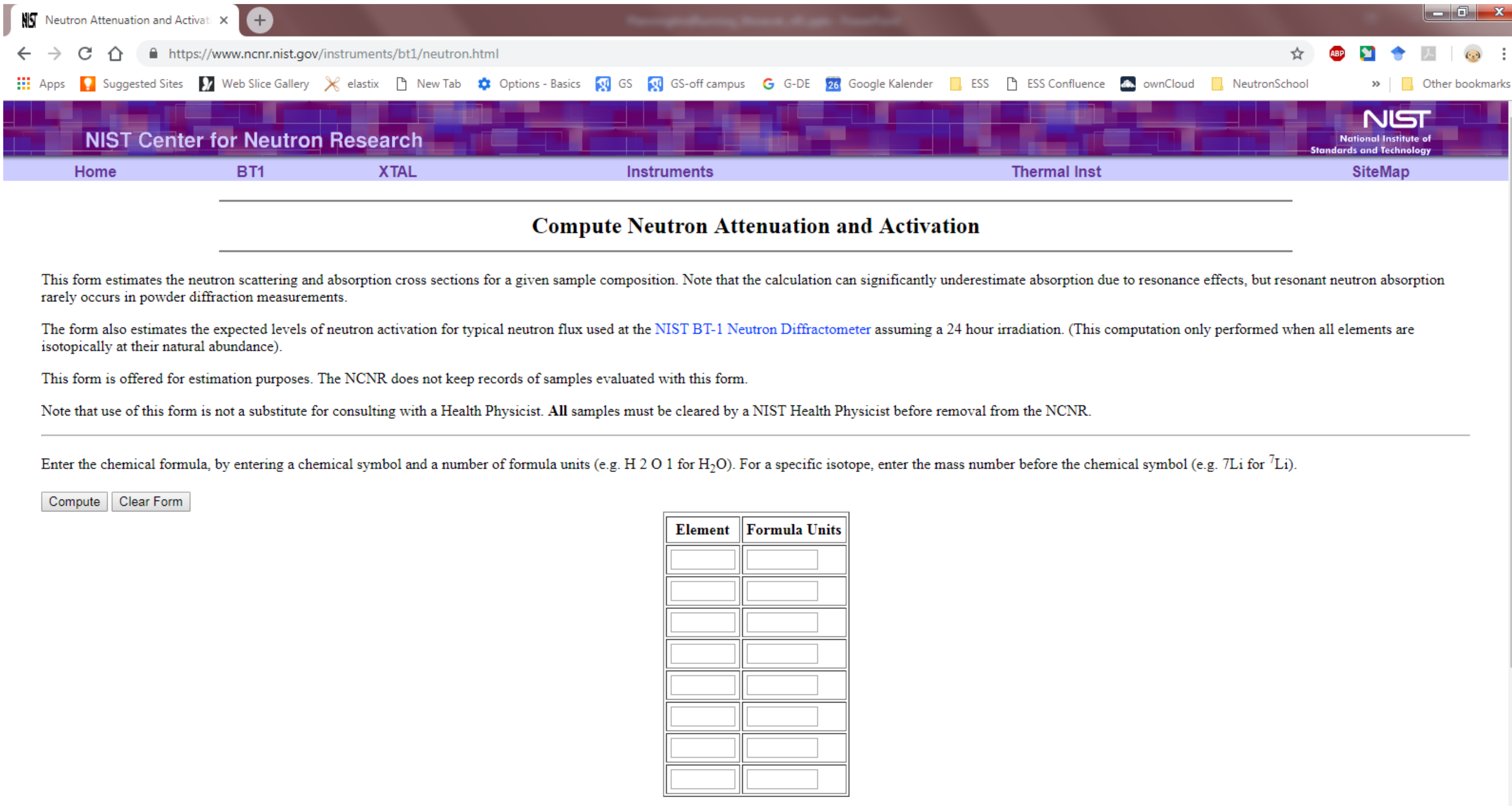
Some useful references

https://www.ncnr.nist.gov/instruments/bt1/neutron.html


Neutron Attenuation and Activat

https://www.ncnr.nist.gov/instruments/bt1/neutron.html

NIST Center for Neutron Research

Home BT1 XTAL Instruments Thermal Inst SiteMap

Compute Neutron Attenuation and Activation

This form estimates the neutron scattering and absorption cross sections for a given sample composition. Note that the calculation can significantly underestimate absorption due to resonance effects, but resonant neutron absorption rarely occurs in powder diffraction measurements.

The form also estimates the expected levels of neutron activation for typical neutron flux used at the NIST BT-1 Neutron Diffractometer assuming a 24 hour irradiation. (This computation only performed when all elements are isotopically at their natural abundance).

This form is offered for estimation purposes. The NCNR does not keep records of samples evaluated with this form.

Note that use of this form is not a substitute for consulting with a Health Physicist. **All** samples must be cleared by a NIST Health Physicist before removal from the NCNR.

Enter the chemical formula, by entering a chemical symbol and a number of formula units (e.g. H 2 O 1 for H_2O). For a specific isotope, enter the mass number before the chemical symbol (e.g. 7Li for ^{7}Li).

Compute Clear Form

Element	Formula Units

AGENDA

- ➢ **Basic considerations ('do the homework')**
- ➢ **How to write a good beamtime proposal**
- ➢ **'Beamtime proposal exercise'**

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The beam time proposal: Administrative

- Inform yourself about the proposal deadlines (typically 2 calls a year)
  - Website of the facilities
  - https://neutronsources.org/
  - Sign up on the mailing list: https://neutronsources.org/mailman/listinfo/neutron
  - International Society for Neutron Radiography (ISNR): https://www.isnr.de/
- Create an user account at proposal system of the facility (start early enough with this)
- All neutron imaging beamlines are typically oversubscribed (factor 2-3)
- respect template, format and length limit
  - reviewers annoyed if proposal not the right format. Proposal might be rejected if not respected.

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The beam time proposal: Basics

- Proposal must be scientifically compelling and competitive!
    - could be done; should be done; must be done; highlights
    - Scientific scientific case? Will neutron imaging give a result which would allow a field to significantly advance?
- highly targeted proposal; avoid vague or too broad aims
    - preliminary measurements or characterization recommended when appropriate
    - have full portfolio requiring now neutrons to provide answers/information on specific point(s)

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EUROPEAN SPALLATION SOURCE

The beam time proposal: Basics

- Lots of proposals!
  - reviewers have many proposals to review and discuss
  - proposal must be self-contained (all important information should be given)
  - reviewers don’t necessarily have time to get extra information from references
  - technically poorly written proposals (typos, errors, non-respect of template and format) have high chance of automatic poor grade
  - structure is important; clear and easy to read
- Consult Beamline Staff
  - target measurements based on beamline (what set-up is needed); clearly identify how your experiment can be done and whether it can give you the answers you need
  - advice on required measurement time (requested days)

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The beam time proposal: the proposal itself

- Proposal Summary
  - probably most important part!
  - equivalent to abstract of scientific paper, one paragraph
  - clear statement on essence of proposal – what are you trying to do, how you intend to do it, and why you are doing it (impact, importance of study)
  - reviewers should understand exactly what the proposal is about from this summary; details are given in the following sections
- Scientific Background
  - set the scene for the interest of your research
  - provide sufficient scientific background to introduce the review committee to the topic (they often not specialists in the particular scientific topic)
  - indicate fundamental and societal importance of your work

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The beam time proposal: the proposal itself

- Scientific Background (*continued*)
  - Describe the hypothesis you want to confirm with the experiment (lead to the open question stated in the summary)
  - refer to any previous measurements or preliminary characterization
  - which information will the experiment provide that can only be obtained using neutron imaging.
  - figure is always useful, can replace many words (general process; previous data to pinpoint problem…)

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The beam time proposal: the proposal itself

- Experiment Details
  - exactly how are you going to carry out the experiment; strategy
  - details and quantity of samples
  - technique and setup; special requirements
  - show reviewers you are ready and prepared
  - allow beamline scientists to make technical feasibility assessment
  - prior discussion with beamline scientist is strongly advised
- Beamline & Beamtime Requirements
  - support the choice of beamline
  - reason for beamtime requested and how this is calculated (table or simple calculation is always good)
  - can be relatively short

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The beam time proposal: the proposal itself

- Results Expected & Significance
    - what results you are expecting
    - how these results will allow you to answer the specific question(s) stated in summary
    - what will be the impact of answering this question on your field of research
- References
    - illustrate importance of topic by citing one or two milestone papers in your field
    - recent exciting developments in or around specific topic of proposal
    - indicate level of your research by citing own recent, relevant publications
    - should not expect that reviewers will have time to read references so all essential information in the proposal!

Planning and running a neutron imaging experiment

At the experiment

- Prepare
  - Start preparation well-ahead of time of the scheduled experiment
  - If in-situ test: make dry-runs in your lab
  - Bring back-up samples if possible
  - Document the samples well (dimensions, weight, number them uniquely)
  - Make a detailed experimental plan: But make it so it can be adjusted! (e.g. an excel sheet with input for #samples, exposure time, # projections, etc)
- Plan
  - Book a hotel/guesthouse close to the beamline
  - Bring enough personnel to help with the experiment
  - Arrive well in advance, plan to stay an extra day(s)
  - Bring harddrives (SSD preferred)

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After the experiment

- How to analyze the data
  - What type of software will you need to analyze the data?
  - If commercial software is needed (e.g. visualization): Check if you can have a follow up visit at the facility and/or of alternative exists
  - If possible, try to get as far as possible while still at the facility
- Beamtime report
  - Important! For the facilities (use of public funding) and for your next proposal!
- Publication
  - Ultimately the goal…
  - Typically the beamline scientist(s) who assisted with the experiment are offered co-authorship

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