Solutions

REMARK: In some places, the exercise text was slightly modified and updated compared to the hand-out.

Exercise 1: Cross Sections for X-Ray Scattering Processes

The interaction of x-rays with matter leads to different processes, namely photoelectric absorption, coherent scattering, and incoherent scattering. These events are strongly dependent on the considered element and are described by different cross sections.
Information on the element-specific cross sections can be obtained from the NIST online database[1]. Fig. 1 shows the behavior of three elements as function of incident x-ray energy.

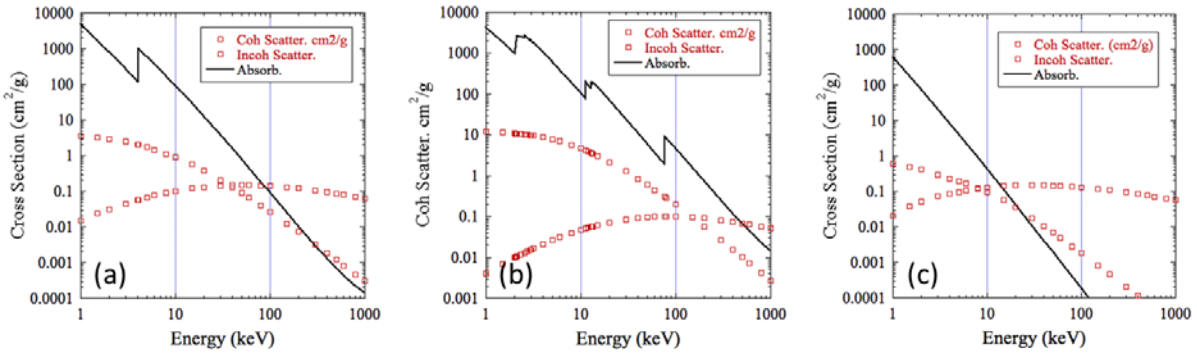


Figure 1. Energy-dependence of photoelectric absorption (black line), coherent scattering (red squares), and incoherent scattering (red squares) for three different solid elements.

1) Why does the photoelectric absorption show discontinuities in some plots? What is the cause for the discontinuities and at which energies do they appear?

   Resonant absorption edges appear at energies that match discrete distances in the electronic energy levels for the specific atoms. K-edges, involving electronic transitions from the innermost (strongest bound) atomic shells show a single step, while L- and M-edges have more structure. For light elements, the excitation energies are too small to appear in this plot (e.g. 13.6 eV for hydrogen).

[1] https://www.nist.gov/pml/x-ray-and-gamma-ray-data, https://gsecars.uchicago.edu/page/xraytable, https://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html.

Away from the resonances, the absorption cross section scales with $1/E^2$, and the absorption is caused by the oscillation of the electrons in the electric field of the x-ray wave, which gets less effective at high frequencies (respective energies).

2) Determine which solid elements corresponds to the shown scattering cross sections.
   (a) Ca (b) Ir (c) Be
3) Which curves represent the coherent and incoherent scattering, respectively? Why?
   The coherent (elastic Thomson) scattering is strongest at low energy, while the incoherent (inelastic Compton) scattering increases with E as an energy transfer to a bound electron becomes more likely.
4) How do the three cross sections depend on the atomic number Z?
   In general, all cross sections increase with the number of electrons, and thus with Z.

Exercise 2: Crystallographic Symmetry and Point Groups

The symmetry of a material describes its invariance under spatial, temporal, and other transformations; and its symmetry group limits the physical characteristics of a material. Here, we want to recall some basic notions of point group symmetry, and its relation to crystallographic and magnetic order.

As a reminder to get warmed up: Point groups consider the transformation under rotations, spatial inversion, roto-inversion operations (e.g. mirror reflections), and time reversal. Use Fig. 2 to recall the transformation of a vector and a magnetic moment (described by a circular current) under the different operations. Regarding nomenclature, spatial inversion $\bar{1}$ = I (**r** → -**r**), and time reversal 1' = T (t → -t).

The trickiest part is the proper transformation behavior of a magnetic moment under mirror operations. Here, it helps to separate the component parallel (μ reverses) and perpendicular (μ stays invariant) to the mirror plane, and visualize the magnetic moment as product of an oriented current loop with a curled hand, and its mirror image with the other.

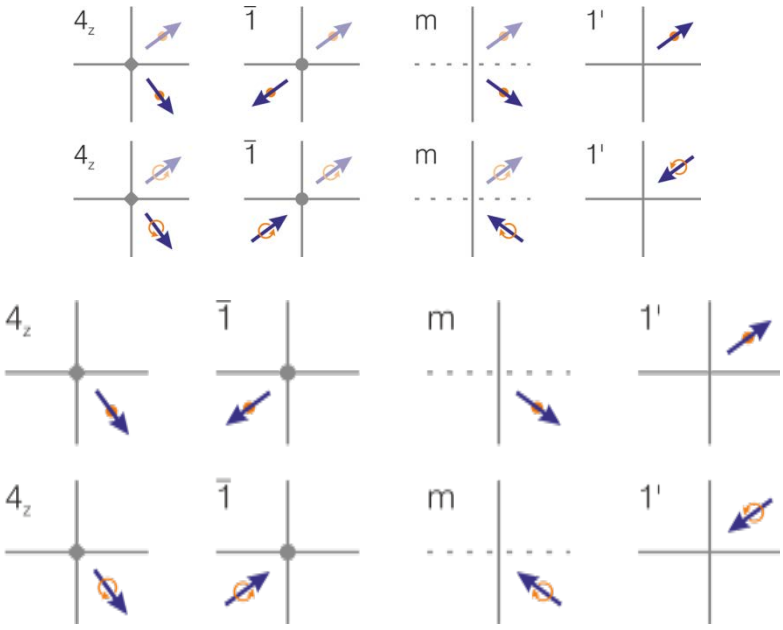
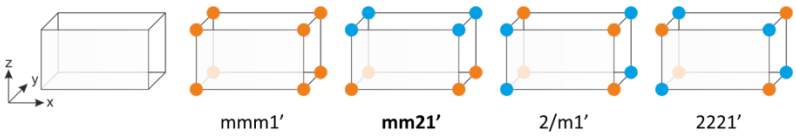


Figure 2. Describe the transformation behavior of a polar vector **r** (top row) and a magnetic moment **μ** (below). Remember that **μ** is an axial pseudo-vector described by an oriented current loop, i.e. **μ** = I**n.**

1) Consider the orthorhombic lattices (with non-magnetic point group mmm1') shown in Fig. 3. Depending on the decoration of the unit cell with different atoms (blue and orange dots), or magnetic moments (arrows) certain transformations are no longer a symmetry operation of the structure.

- Cross out those operations that are no symmetry element of the decorated structure, assuming the centre of symmetry in the centre of the cuboid! Can you name the resulting point group?

Answer:

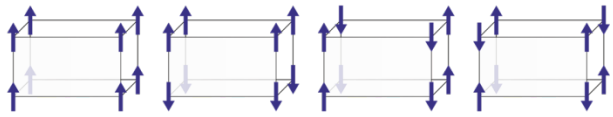


(a) $1, 2_x, 2_y, 2_z, \bar{1}, m_x, m_y, m_z$

(b) $1, \cancel{2_x}, \cancel{2_y}, 2_z, \cancel{\bar{1}}, m_x, m_y, \cancel{m_z}$

(c) $1, \cancel{2_x}, \cancel{2_y}, 2_z, \bar{1}, \cancel{m_x}, \cancel{m_y}, m_z$

(d) $1, 2_x, 2_y, 2_z, \cancel{\bar{1}}, \cancel{m_x}, \cancel{m_y}, \cancel{m_z}$



(e) $1, \cancel{2_x}, \cancel{2_y}, 2_z, \bar{1}, \cancel{m_x}, \cancel{m_y}, m_z, \cancel{1'}, 2'_x, 2'_y, \cancel{2'_z}, \cancel{\bar{1}'}, m'_x, m'_y, \cancel{m'_z}$

(f) $1, 2_x, 2_y, 2_z, \cancel{\bar{1}}, \cancel{m_x}, \cancel{m_y}, \cancel{m_z}, \cancel{1'}, \cancel{2'_x}, \cancel{2'_y}, \cancel{2'_z}, \bar{1}', m'_x, m'_y, m'_z$

(g) $1, 2_x, 2_y, 2_z, \bar{1}, m_x, m_y, m_z, \cancel{1'}, \cancel{2'_x}, \cancel{2'_y}, \cancel{2'_z}, \cancel{\bar{1}'}, \cancel{m'_x}, \cancel{m'_y}, \cancel{m'_z}$

(h) $1, \cancel{2_x}, \cancel{2_y}, 2_z, \cancel{\bar{1}}, m_x, m_y, \cancel{m_z}, \cancel{1'}, 2'_x, 2'_y, \cancel{2'_z}, \bar{1}', \cancel{m'_x}, \cancel{m'_y}, m'_z$

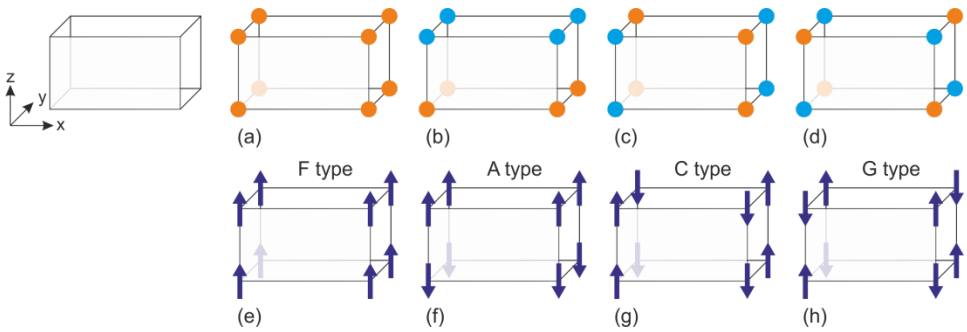
- Which structures do have the right symmetry to allow for ferroelectricity (i.e. a spontaneous electric polarisation)?

  Only the point group mm21' has a polar axis (i.e. a direction with different "ends") and thus allows a spontaneous polarisation. In the case of 222 the spatial inversion is broken as well, but there is no polar axis, instead the system has chiral symmetry.

- How would the modified symmetry affect the scattering pattern?

  For the magnetic decoration, the translational symmetry and Laue group remain unchanged, but the peaks in the diffraction pattern will gain (a) more intensity to the ordered moments, and (b) relative intensities will differ.

  The orthorhombic groups mmm, mm2, and 222 have the same Laue group and the scattering patterns will not differ (unless one makes a detailed investigation of Friedel pairs to detect the lack of an inversion centre). Here, additional "conventional" experiments, e.g. non-linear optics, can help resolve the point group. The decoration with symmetry 2/m has a different crystal class, and additional reflexes can arise in the scattering pattern.



(a) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z$
(b) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z$
(c) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z$
(d) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z$
(e) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z, 1', 2'_x, 2'_y, 2'_z, \overline{1}', m'_x, m'_y, m'_z$
(f) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z, 1', 2'_x, 2'_y, 2'_z, \overline{1}', m'_x, m'_y, m'_z$
(g) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z, 1', 2'_x, 2'_y, 2'_z, \overline{1}', m'_x, m'_y, m'_z$
(h) $1, 2_x, 2_y, 2_z, \overline{1}, m_x, m_y, m_z, 1', 2'_x, 2'_y, 2'_z, \overline{1}', m'_x, m'_y, m'_z$

Figure 3. Orthorhombic lattices (point group mmm1'), with different decorations. Below: Symmetry operations of the orthorhombic point group mmm1', strike out operations that are not symmetry operations of the decorated lattices.

Exercise 3: Analysis of Scattering Patterns

Scattering patterns contain a wealth of information. Here, we want to discuss several aspects of scattering patterns in relation to the underlying physical properties of the investigated material.

1) In general, what information can be extracted by the
   - position of the scattering peaks,
     Translational symmetry (Bravais lattice) and rotational symmetry (point groups) => space groups; relative distances: lattice periodicities
   - the peak intensity,
     Systematic absences: Bravais lattice (centring), glide planes and screw axes
     Accidental absences and relative intensities: different atomic species
   - and the peak widths?
     Peak width contains information about crystallite size, correlation length, and disorder. Also strain in the material can be measured.
   - What information can be hidden in the background of a scattering pattern?
     Diffuse scattering can contain information on short-range correlations (e.g. magnetic), and disorder present in the system.
2) Non-primitive translational symmetry i.e. Bravais lattices, can lead to systematic absences of scattering peaks in a diffraction pattern. Here we consider the three space groups Pm3m, Fm3m, and Im3m that have the same cubic point-group symmetry. Fig. 4 shows simulated Laue patterns for each of these cubic space groups.
   - How does the translational symmetry of the lattices differ?
     Bravais lattices describe the relationship between the lattice vectors defining translational symmetry. P = primitive, F = face-centred, I = body-centred (German "innen-zentriert"). Furthermore, base-centred (A,B,C) Bravais lattices are possible.
   - Along which crystallographic axis is the cubic crystal viewed?
     From the symmetry of the scattering pattern, one can conclude that the line of sight (German "Blickrichtung") is along the three-fold space diagonal 111.

- Relate the simulated[2] Laue patterns to the different space groups. Use the conditions for allowed reflections[3] stated in Tab. 1.

  The easiest space group to assign is the Pm3m structure with primitive cell. Here, reflections are not constrained and the respective scattering pattern is the one in the middle of Fig. 4.
  Left scattering pattern = Im3m. Here, the reflections indexed with 112, 323, 255, 233, 103, and 211 obey the respective selection rules. However, for the 551 reflection the rules for Fm3m is correct, and the peak at 225 is not allowed by either space group.
  Right scattering pattern = Fm3m. The reflections at 313, 537, 133, and 311 obey the respective rules. However, this is not true for peaks at 225, 354, and 221.
  Why are there deviations from the expected behavior?

- What other space-group symmetries can lead to systematic absences?

  Glide planes and screw axes. Furthermore, accidental absences can occur if atomic form factors are similar in magnitude (also see Exercise 4.4).

	Pm3m No. 221	**Fm3m** No. 225	**Im3m** No. 229
hkl	No conditions.	*h+k, h+l, k+l = 2n*	*h + k + l = 2n*
0kl		*k, l = 2n*	*k + l = 2n*
hhl		*h + l = 2n*	*l = 2n*
h00		*h = 2n*	*h = 2n*

Table 1: Conditions for allowed reflections for different cubic space groups. The indices *h*, *k*, *l* are permutable. From the International Table of Crystallography. REMARK: Please note that on the exercises I mistakenly wrote "systematic absences" in the caption – of course, the conditions for *allowed* reflections are shown here!

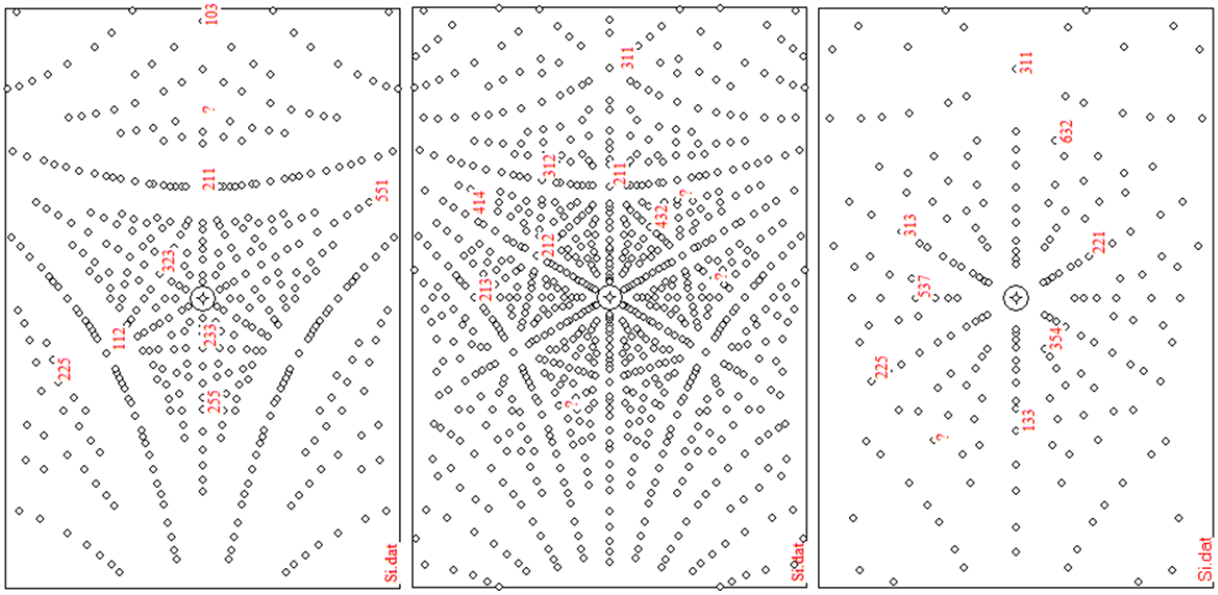


Figure 4: Laue diffraction patterns for different cubic space groups (simulated with OrientExpress). Selected peaks are indexed with their respective hkl values.

[2] OrientExpress: https://www.ill.eu/instruments-support/computing-for-science/cs-software/all-software/orientexpress/
[3] International Tables for Crystallography: http://it.iucr.org/. A good introduction can be found in "Space groups for solid state scientists" (M. Glazer, G. Burns, and N. Glazer, Academic Press, 2013). Also, useful tools can be found on the Bilbao server, e.g. conditions for reflections http://www.cryst.ehu.es/cryst/get_hkl.html.

Exercise 4: Method Comparison

1) Derive the equation relating the wavelength (in Angstroms) to the energy of x-rays, electrons, and neutrons (in all cases consider the energy given in eV).

   Classical particles, using de-Broglie formula: $\lambda = h / \sqrt{2*m*e} * 1/\sqrt{U}$. Light: $\lambda = h*c/e * 1/U$. λ_e [Å] = 12400 / sqrt(E [eV]), λ_n [Å] = 0.286 / sqrt(E [eV]), λ_γ [Å] = 12.2 / E [eV].

2) The relationship of λ(E) for electrons, neutrons, and x-rays is summarized in Fig. 5. Assign the different particles to each curve! What is the reason for the different slopes? What particular scales do the shaded regions correspond to?

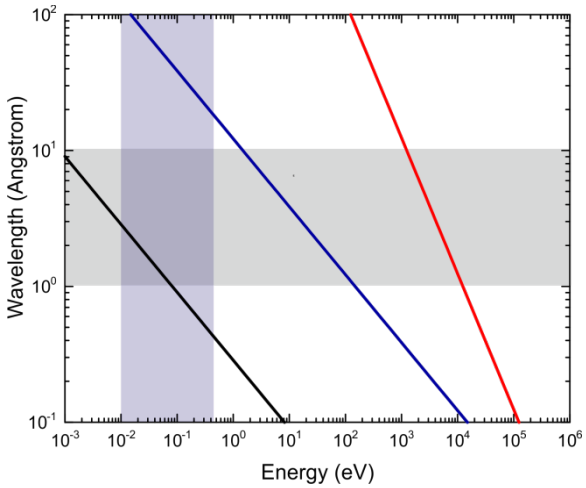


Figure 5: Relationship between energy and wavelength for different probes.

From left to right: neutrons, electrons, x-rays. Non-relativistic particles have square root dependence between energy and wavelength, while light has a linear relationship. The grey region corresponds to wavelengths comparable to atomic distances and periodicities found in crystals, the blue region roughly marks the energy of collective excitations, such as phonons and magnons.

3) Consider the atomic form factor for Co seen by neutrons, electrons, or x-rays (Fig. 6).
   - What do the different probes interact with, and how does the shape of the scattering potential affect the angular intensity distribution?

     Neutrons interact mainly with the atomic nucleus (and the magnetic moment in the electron shell), x-rays interact with the electrons, while electrons interact with both the electrons and the nucleus. Dependent on the relationship between particle wavelength and extension of the scattering potential the scattering can be described by point-source scattering without angular dependence (i.e. neutrons). In case of electrons and x-rays the interaction of the extended electron shell leads to a pronounced angular dependence of the scattering.
   - What does determine the value f(0) at zero angle (red and yellow points)? Where can you find the respective values?

     For x-rays the atomic form factor at zero is equal to Z. For neutrons the form factor is a non-monotonic function of Z and determined by the internal structure of the nucleus (isotope-dependent!). It can only be measured by experiment (see Neutron Data booklet[4]).
   - How does the form factor changes for heavier atoms probed by x-rays?

     The atomic form factor is the Fourier transform of the electron density surrounding the atom. Therefore, as Z increases, the maximum value f(0)=Z increases and the potential gets steeper and more narrow as the electron cloud gets larger.

[4] Neutron Data Booklet: https://www.ill.eu/fileadmin/users_files/documents/links/documentation/NeutronDataBooklet.pdf

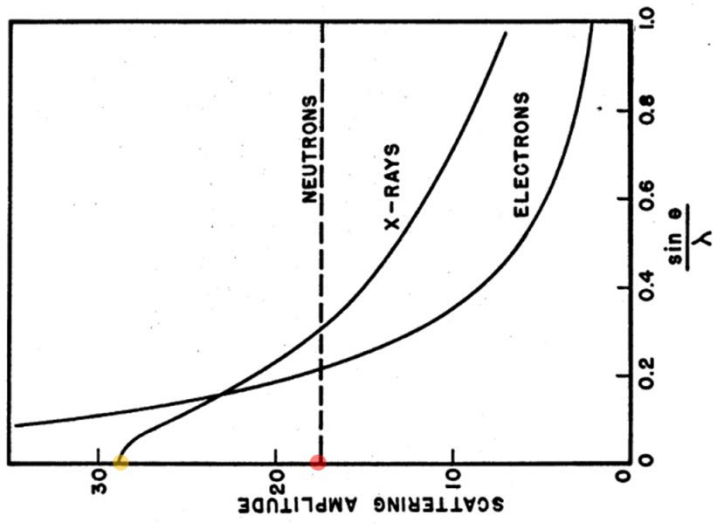


Figure 6: Atomic form factors of copper for x-rays, electrons, and neutrons. From Science **108**, 69-75 (1948).

4) Fig. 7 shows two powder scans for KCl, one of which was measured with x-rays and the other with neutrons of the same wavelength. Which plot was measured with x-rays and which one with neutrons? Describe and explain the differences.

All reflections of diagram (a) also do appear in diagram (b) at the same diffraction angle, but diagram (b) also shows additional reflections. The intensity of the reflections of the NaCl structure depends on the sum or the difference of the two atomic form factors (x-rays) respectively scattering length (neutrons). As $f_K \approx f_{Cl}$ (since Z differs only by 2!) some peaks will be almost completely extinguished, while this is not the case for neutrons with $b_K \neq b_{Cl}$. Therefore, the left diagram is obtained from x-ray diffraction and the right one using neutrons. In addition, in the left diagram the scattering intensity falls off much faster with the scattering angle than in the right diagram. This reduction is due to the angular dependence of the atomic form factor. In contrast, the neutron scattering length is independent of the scattering angle.

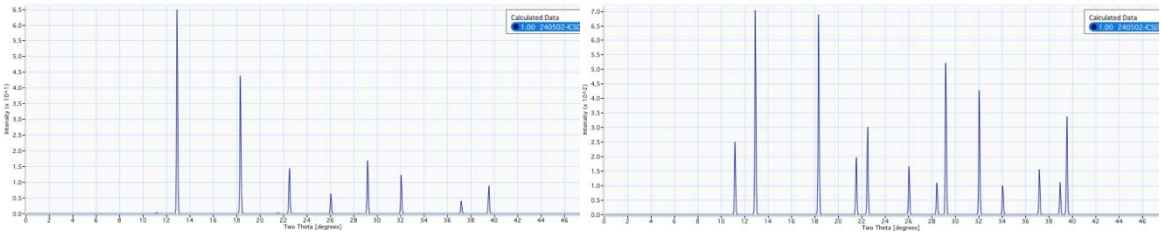


Figure 7: Powder diffraction patterns of KCl measured with neutrons and x-rays.

5) Discuss for the following problems the suitability of x-ray and neutron methods.

- Quantitative determination of overall structure.

  X-ray: Well-suited. The intensities can be measured with high precision and comparatively small effort using a table-top experimental setup. Data evaluation usually is problem-free.

  Neutrons: Experiments need to be performed at large-scale facilities (reactor or spallation source), where measurement time is rationed. Due to the weak matter-neutron interaction investigated crystals need to be substantially larger (~mm^3) than for x-ray analysis (50-500 μm^3). Data evaluation is comparable to the x-ray case.

  Electrons: Due to the strong interaction of electrons with matter, dynamic scattering theory must be used to evaluate the data. This makes the structural analysis complicated and error-prone. Exceptions are transmission electron microscopy (TEM), which allows for a direct

imaging of the atomic structure or the reciprocal lattice of small areas of the sample – but preparation of TEM samples is elaborate.

- Information from nanoscale crystallite and/or nanoparticles.

  X-rays and neutrons: It is practically impossible to focus the beam down to nanometer dimensions. Furthermore, the intensity scattered from nanoparticles is generally too weak to be measured with sufficient accuracy. However, powder samples of nanocrystals can be investigated with x-rays and neutrons, and also imaging x-ray imaging methods such as PEEM and STXM are valuable tools to investigate nanoscale materials.

  Electrons: Electron beams can be focused down to a few nanometers, and the strong electron-matter interaction leads to sufficiently high diffraction intensities.

- Surface analysis.

  X-rays and neutrons: Neutrons and hard x-rays have great depth penetration in matter and are therefore of limited use for surface analysis. However, dedicated techniques have been developed to allow for surface sensitivity such as x-ray grazing incidence diffraction and photoemission electron microscopy (PEEM). Furthermore, soft x-rays are strongly absorbed, and thus yield information of surface properties.

  Electrons: For low-energy electrons, the penetration depth is only a few Ångström. (Backscattered) electrons therefore show almost exclusively the surface properties of the analyzed material. Note that a transmission electron microscope (TEM) with an applied voltage of 200 kV can travel through 100 nm of sample thickness.

- Isotope analysis.

  Neutrons win this one, since the atomic form factor depends in a non-monotonic fashion on the number of neutrons and protons in the nucleus (see Neutron Data Booklet).

- Chemical composition of the material and the matrix.

  X-rays: Possible with x-ray spectroscopy methods (WDX, EDX).

  Electrons: Use electron energy loss spectroscopy (EELS).

  Neutrons: Due to the weak interaction with most specimens a chemical analysis is rather difficult to perform with neutrons. However, the neutron contrast between light elements is heavily used for the investigation of polymers and biological samples.

- Determination of biological structures (proteins, viruses etc.).

  X-rays: Well-suited. As biological structures are gradually destroyed by x-rays (creation of radicals), short experiments using high-intensity beams (synchroton sources) are advantageous.

  Electrons: Electron bombardment destroys biological specimens rather quickly. Better electron imaging requires metallized samples, thus in-vivo measurements are (nearly) impossible.

  Neutrons: Well-suited. Due to the weak interaction with matter, neutrons do not destroy biological structures. However, because of this weak interaction, it is necessary to use very big crystals (several mm^3), that can be difficult to grow.

- Nondestructive analysis of large specimens (1 cm^3 and larger).

  Neutrons can pass through specimens of several cm thicknesses, while absorption limits x-rays transmission experiments severely.

- Analysis at extreme temperatures and pressures.

  X-rays: Suited. However, instrument design is more complex. Because pressure-and heat-resistant materials are usually made of heavy elements, the equipment will interact strongly with x-rays and thus negatively affects the experiment.

Electrons: Less suited than x-ray and neutron experiments. The specimen must be placed in high vacuum and additional material in the beam path (e.g. pressure cells) will fully absorb the beam. Heating and cooling via a cold finger sample holder is nevertheless possible.
Neutrons: Very well suited, because ovens, cryostats and pressure can be built to be almost transparent to the radiation (using suitable materials).

- Determination of the phonon or magnon spectrum of a crystal.
  X-rays and electrons: As x-ray photons and electrons possess a much higher energy than phonons (see exercises 4.1 and 4.2), energy losses and gains from inelastic scattering by phonons barely can be measured. However, specialized synchrotron experiments and recent machine development permit a resolution of the phonon spectrum (e.g. RIXS, ultrafast x-ray diffraction).
  Neutrons: With a wavelengths in the range used for structural determination (≈1 Å) the neutron energy is comparable to that of phonons. Inelastic neutron scattering therefore allows determination of the phonon energies and thus their spectrum.

Exercise 5: Planning an Experiment at a Large-Scale Facility

Due to the complexity and rarity of large scale facilities, experiments using synchrotron, neutron, or muon sources usually require quite an amount of preparation, and the analysis of the acquired data can also take a prolonged amount of time. Therefore, careful planning of the different steps in the research chain (see Fig. 8) helps to achieve the best result, may avoid problems, and minimises risks.

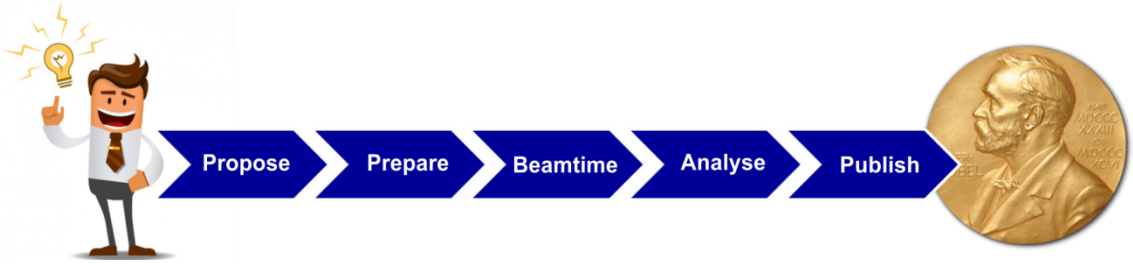


Figure 8. The research chain

In this exercise we will split into five groups, each of which will tackle a different stage of the research chain (see short description of each task below). Think of all possible small and large tasks associated with the different steps – you need to plan for what, where, when, who, and how. What could go wrong, and how could you prevent mistakes? What could you do to be more successful? Almost all experiments are collaborations – how do you best communicate and work with your colleagues?

Discuss, and write down tasks associated with each stage (one task per sticky note, use a thick marker). We will collect all ideas, and discuss the stages together with the group.

1. **Proposal:** Eureka! You have a wonderful idea for a highly unusual experiment, and your colleagues agree that you should apply for beamtime to perform the measurements at PSI. The deadline for submission is soon – how do you write a successful proposal?
   - Communicate with (potential) co-proposers and beamline scientists (or people who know the beamline well). Don't be afraid to ask people you don't know personally, many people are happy to help, but don't expect last-minute wonders – be early rather than late!

- What exactly do you want to find out (be specific)?
- Literature search: Has it been done before? Current knowledge? What is new?
- How to measure? What is a good probe? Suitable beamlines? Specifications of sample environment (minimum and maximum sample sizes)? Limitations of beam properties? Sensitivity and q-range of instrument
- Preliminary experiments available? Contact beamline scientist to discuss requirements?
- When is proposal deadline? Assessment criteria? Formatting requirements? Length of text – how many pages maximal, allowed number of citations, allowed number of figures? Check out submission procedure (webpages might crash shortly before a deadline!). Name funding sources. In case biological, chemical, or hazardous materials are used ensure transport, storage, and experiment are possible.
- Team building and distribution of roles and responsibilities. Agreement with co-proposers?
- Proposal submission and acceptance. When will be beamtime scheduled if proposal is accepted (who would join the experiment)?

2. **Preparation:** Congratulations! Your proposal got accepted, and you've got granted 12 shifts (à eight hours) of beamtime in four months' time. What do you have to prepare now in order to be able to perform a successful experiment?
    - Simulate and describe expected result as best as possible.
    - Beamtime scheduling – safety training, dosimeter, book accommodation and travel… Who pays for this?
    - Sample growth and preparation (orientation, polish, …). Sample transport and deliveray (sample must arrive before or on time, have a letter of reference from a professor with you in case you get asked in customs). Have backup samples ready!
    - Characterisation (structure, magnetisation, phase transitions, …).
    - Where to get healthy food during the beamtime (including weekend and night shifts)?
    - Who will help with sample preparation, simulations/theory, and during the beamtime? Are enough people ready for the experiment? What do you do in case somebody drops out on short notice (visas, safety clearance, and pre-training might be required in some places)?
    - Make an experimental plan, on what to measure, which parameters to test, how much time will be required for each step (and leave buffer time at the end). Prepare a template to document the experiments (i.e. a lab-book with prepared forms – but be ready to overthrow it if the format does not work for you!).
    - Sample stage/mounting: In case of non-standard experiments, make sure any additional equipment (mechanical, electrical, etc.) is ready, and fits to the beamline. Also, don't forget any other equipment you might need during the beamtime that is not available at the beamline (e.g. tweezers, gloves, glue, …).
3. **Experiment/Beamtime:** You arrive at PSI for your 12-shift beamtime. What will you do the next four days, and how do you make sure to get the best results out of your experiment? How can you best avoid problems during your beamtime?
    - Introduction by beamline scientist, how to use the instrument, how to use the sample environment (cryogenics, sample replacement). Who is able to do what – are they around at the critical times (technicians and beamline scientists might have regular hours and weekends)?
    - Time management: Who will do which shifts? Can one run batch scripts, or should someone always stays with the experiment? What is the measurement plan (specifying samples, parameters, measurements, time requirement) – plan also for buffer time, and re-assess the plan during the beamtime.

- Analyse data on the fly, if possible – did you choose the correct parameters, does the sample work, do you need to change something?
- How to make sure that communication works even in the case of night-shift hand-overs? Are there ideas how to keep the lab book? Also write down even small details – they might be important later!
- Beforehand & during: Communicate experimental plan, objectives, and backup plans.
- Communication in the measurement team – especially at shift turnover?
- If something goes wrong: Don't panic – Stop and Think! And be nice to each other!
- After beamtime: Save data, and copy the lab book.

4. **Data Analysis:** You slept off your jetlag and you finally are awake enough to look at your measurements in detail. How do you analyse the data obtained at the beamtime, and what tools are available to you?
    - How the data is stored, how to access data? Can data be copied? Backup the data!
    - Review the data after the beamtime, before a proper analysis (e.g. make a table of all useful measurement series and considered parameters to analyse later). Check if the numbers make sense with respect to the sensitivity of the experiment. Define statistical errors.
    - What are resources to read and analyse data? Data format?
    - Analysis, *discussion*, theoretical models, simulations
    - Interpretation of data, with respect to theory, simulations, available literature
    - Do additional measurements (new proposal needed?)
5. **Publication:** Great! You finally understand your data. Now you need to publish your results – how do you get on writing the manuscript? Who should know about your work, and how can you make sure they learn about your discovery?
    - Submit a beamtime report (usually one page)!
    - Relate to concepts and results known in literature (literature review and search).
    - Prepare figures and text, storyline, supplementary materials (if needed).
    - Discuss! Get agreement from collaborators and acknowledge all contributions to the work (technicians, service jobs, funding sources, etc.).
    - After internal review process: Write letter to the editor, submit, (hopefully not resubmit), give feedback to peer review, read proofs. Publish. Before even submission you might want to upload your contribution to a preprint server like www.arXiv.org to ensure your original contribution is acknowledged (especially in highly competitive areas) and to make your results available without a paywall.
    - After publication: Write statement for public relations. Present your results at conferences.

    Rinse and Repeat. And keep up the good work ☺

Exercise 6: Designing a Beamstop for the SwissFEL Free Electron Laser

Free electron lasers produce short x-ray pulses with extremely high intensity. In this exercise we consider the particular properties a beam dump designed to stop such a beam has.

1) What is the power (in Watt) of a 10 keV x-ray beam with 10^{11} photons/second?
   $Q = E / t = 10\ \text{keV} * 10^{11} / 1\ \text{s} = 1.602 * 10^{-19} * 10^{4} * 10^{11}\ \text{J/s} = 0.16\ \text{mW}$
2) The specific heat of copper is $C_v = 0.384\ \text{J/(g·K)}$. The density of Cu is $\rho = 8.92\ \text{g/cm}^3$. The X-ray beam is dumped into a 1 mm^3 Cu block we use as a beamstop. Calculate the temperature rise (in K/s) for a 10 keV x-ray beam with 10^{11} photons/s.

$\Delta T = Q / (C_v * m)$ $Q = 0.16$ mW $m = V * \rho = 8.92 * 10^{-3}$ g
$\Delta T = 0.16$ mW / (0.384 J/(gK) * 8.92 mg) = 0.047 K/s

In contrast to synchrotrons, which can be regarded as continuous sources; free electron lasers generate x-ray pulses of 100 fs length with typical repetition rates of about 100 Hz. This means that all of the ~10^{11} photons arrive in a very short amount of time, and the material of the beamstop will be under stress, as the x-ray excitation is faster than the heat propagation. Therefore, the considered volume of heat-dissipation is not given by the size of the beamstop, but rather by the beam diameter (eg. 20 μm) and the x-ray absorption length for that specific material and x-ray energy (here Cu@10keV).

3) Calculate the temperature rise in this case. Would you be able to use a beamstop designed for a synchrotron in an x-ray free electron laser?

   The absorption coefficient can be obtained from the NIST database (see Exercise 1), and is approximately $1.8*10^3$ cm^{-1}. The absorption length is its inverse, i.e. about 5.6 μm.

   https://physics.nist.gov/cgi-bin/ffast/ffast.pl?Formula=Cu&gtype=5&range=U&lower=9&upper=11&density=8.92

   $Q = E / t = 10$ keV $* e * 10^{11} * 100$ Hz $= 16$ mW

   $V = 5.6 * 10^{-6} * \pi * (10 * 10^{-6})^2$ $m^3 = 1.8 * 10^{-15}$ $m^3 = 1.8 * 10^{-9}$ cm^3

   $m = \rho * V = 16.0 * 10^{-9}$ g

   $\Delta T = Q / (C_v * m) = 2.6 * 10^6$ K/s

4) Discuss the influence of the beam size on the temperature increase.

   The temperature rise is inversely proportional to the illuminated area, $\Delta T \sim 1/A$, and thus heating will be reduced for a larger beam diameter.

Exercise 7: Electricity Bill of the Swiss Light Source

In this exercise we will make a qualitative estimate of the amount of energy and power required to run the SLS storage ring as well as its electricity bill. Simplifying the problem, the energy required to run SLS can be divided in three parts:

1) **The energy required to accelerate** the electrons to relativistic speeds.
   - Calculate the energy required to accelerate the electrons to a speed v=0.99c. Upon acceleration an electron gains a kinetic energy of $K_E = (\gamma-1)m_e c^2$, where $\gamma = 1/\sqrt{1-(v/c)^2}$ and we need to accelerate enough electrons to sustain a current of 400 mA in the storage ring.

     For v = 0.99c one gets $K_E = (\gamma-1)m_e c^2 = 3$ MeV = 4.9e-13 J.
   - The final energy in the SLS storage ring is 2.4 GeV, calculate the electron speed v as they travel in the ring.

     Reversing the formula for K_E given above yields: $v/c = (1 - (K_E/mc^2 + 1)^{-2})^{0.5}$.

     For $E_K = 2.4$ GeV one gets $v = 0.999\,999\,977$ c.

2) **The energy radiated** by the electrons while they are circulating in the storage ring (which should be continuously replenished). Calculate the power radiated by the electron while circulating in the storage ring. Use the following formula: $P_{rad}[kW] = 1.266 \cdot E_{SR}[GeV]^2 \cdot B^2[T] \cdot L[m] \cdot I[A]$, where E_{SR} is the energy of the electron in the storage ring, B=1.4 T is the magnetic field used to steer the electron beam, $L = 2\pi r_B$ is the total length of the deflecting sections and I=400 mA is the electron

current in the storage ring. r_B is the bending radius of the dipole magnet and can be estimated by the ratio r_B [m] = 3.3·E_{SR} [GeV]/B[T].

Number of electrons in the ring: $I = ne/t \rightarrow n/t = I/e = 2.5 * 10^{18}\ s^{-1}$

$r_B = 5.66$ m $L = 35.55$ m

$P_{rad} = 1.266 * 2.4^2 * 1.4^2 * 35.55 * 0.4 = 203$ kW

3) **The energy required** by the power supplies that make the synchrotron work, for example creating the strong fields in the bending magnets of the storage ring.
   - Estimate from Fig. 9 the power required during SLS operation.

     Sum up power consumption of all components when the beam is fully ramped up:

     P = (140 + 480 + 740 + 780) kW = 2140 kW.
   - How does this energy consumption relate to the power dissipated by the bremsstrahlung of the electrons orbiting in the storage ring?

     The loss by bremsstrahlung is almost 20 % of the power required to keep SLS running, and these losses must be compensated to keep a continuous beam in the storage ring.
4) The yearly SLS operation time is given by 5000 hours of user operation, 1000 hours of beamline development, and 800 hours of machine development. Consider an electricity price of 0.12 CHF/kWh.
   - Calculate the annual electricity bill of the SLS.

     6800 h * 2140 kW * 0.12 CHF/kWh

     ~14.55 GWh * 0.12 CHF/kWh

     ~ 1.7 MCHF.
   - What is the major source of expenses in running a synchrotron?

     The high-frequency generators needed to accelerate and compensate radiation losses require the most power.

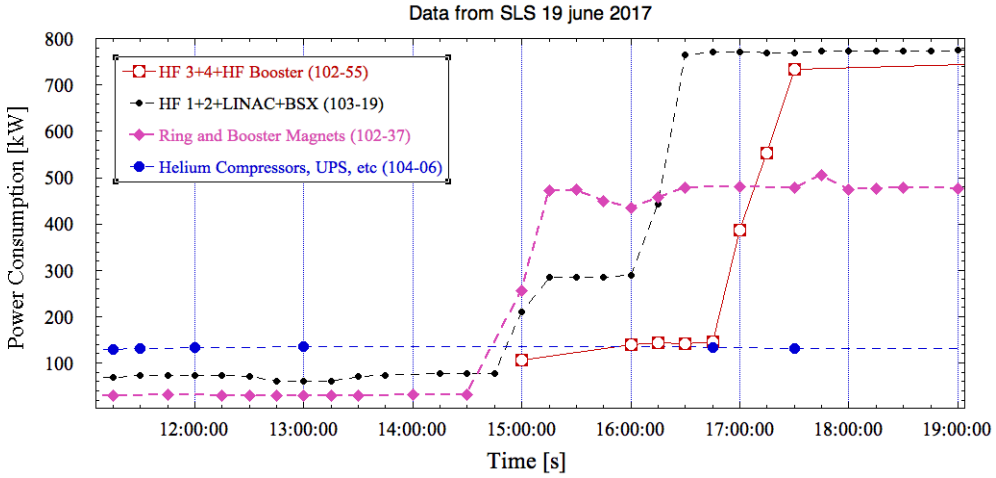


Figure 9: This plot illustrates the change in the absorbed power during the filling of the storage ring as measured at four different transformers that feeds different elements of the SLS machine. The blue line describes the power required by the "services" such as UPS (Uninterruptible Power Supply), vacuum pumps and cryogenic devices (e.g. helium compressors). The purple line describes the power required by the bending magnets in the booster and in the storage ring. The blue line describes the power required by radiofrequency (RF or HF in German) structures HF1, HF2 and the LINAC RF that create an intense electric field required to accelerate the electrons. The red line describes the power

required by HF3, HF4 and HF Booster. According to the plot, after the injection of the electrons, which starts around 14:30, a stable electron beam is obtained around 18:00.