Diffraction and imaging simulation Lab
Laboratory exercise 2
TFY4255 Materials Physics 2024
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Introduction

(Fast) Fourier transformations ((F)FTs) illustrate the basic ideas of reciprocal space and diffraction. Furthermore, FFT can show the link between diffraction and imaging and image processing. In this lab exercise "simulations", you will explore how FFT can be useful. The main goals are, by using simple coding, i) visualize and better understand both the relation between real and reciprocal space, ii) how diffraction can be used to distinguish different structural aspects and iii) use and reflect on theory presented in lecture & book.

Unlike the other lab exercises, you can do this exercise in your own time, and the scheduled lab slot is as an hour where you can ask questions/support and discuss. Therefore, before the scheduled lab slot, we highly recommend that you try to perform the tasks by yourself or together with a lab partner. It is highly recommended to read the background literature [1].!

You need a basic understanding of python to execute the exercise. However, the focus should be on physical interpretations of the studied phenomena and the effects of different structural parameters. Therefore, you are provided with a template code written in Python 3 and example images via [2]. You can use the code via a Juypterlab [2], which requires no python installation on your own PC or your own local python environment. You are free to choose the format you prefer, to write your own independent code, or to modify the provided code in any way you find convenient. Be alert, what a cell does and what is plotted (ie. optimize, correct when required). You are also free to use images of your preference, but at this NTNU separate files cannot be larger than 800 kB. If you write your own code or adapt the given code essentially, include the used code in an appendix in your report. The general report requirements are explained in a separate document and make use of what you learned from writing Lab1 report.

Diffraction from one dimensional crystals

Consider a one-dimensional (1D) crystal with atoms centered at $R_n = na,$, for atom $n \in N$, where N is the total number of atoms. The electron density of each atom can be modelled by a Gaussian with amplitude A_n and width σ_n. The total **electron density**, $\rho(x)$, is then given by

$$\rho(x) = A_n \sum_{n=1}^{n=N} e^{\left(-\frac{(x-R_n)^2}{2\sigma_n^2}\right)} \quad (1)$$

For kinematical diffraction, the scattering amplitude, $F(q)$, is given as the FT of the electron density of the crystal,

$$F(q) = FT(\rho(x)) \quad (2)$$

The diffraction pattern (or diffractogram) of the crystal shows the distribution of scattered intensity. The **intensity** is described by

$$I(q) \propto |F(q)|^2 \tag{3}$$

The intensity of the peaks in the diffraction pattern scales as $I(q) \sim N^2$, while their width is inversely proportional to the number of atoms ($\propto \frac{1}{N}$). For a perfect, endless crystal, the diffraction pattern consists of δ-functions located at the reciprocal lattice points.
If the crystal has a **monoatomic basis**, all atoms have the same atomic number, and the electron density, ρ, will have the same magnitude, A_n , and width, σ_n, for all atoms, i.e. for all n. A **diatomic basis** on the other hand, consists of two different atom types, which can be modelled for instance by letting the amplitudes, A_n, and/or widths, σ_n, of the Gaussians take one value for even n and another for odd n.
At finite temperatures, the atoms are moving about their lattice positions, which can affect the intensity distribution in the diffraction pattern. A simple way of including **thermal motion** in the model, is to add a random number $\alpha_n \in (-1,1)$ that is multiplied by a factor ε to each atom position, so that

$$R_n = na + \propto_n \varepsilon \tag{4}$$

Statistically disordered (amorphous) materials with no long-range order, e.g. glasses, different from noise and thermal motion, can be modelled by letting each atom position vary cumulatively with respect to the neighbouring atom positions, rather than with respect to an invisible ideal lattice. The atom positions in such a model are given by

$$R_n - R_{n-1} = a + \propto_n \varepsilon_g \tag{5}$$

where ε_g determines the upper and lower limits of the positional fluctuations. Note the difference between the structures described by (4) and (5). The varying atom positions and electron densities are reflected in the observed intensities. You should alter structural parameters (eg. model, A_n, σ_n, α_n, N) and related them to calculated variations in I(q).

Fast Fourier transformations and imaging
FFTs are useful for illustrating diffraction. The FFTs of images of objects are closely related to the diffraction patterns obtained from the same objects. Computing an FFT of an image is a mathematical operation where the image is expressed as weighted periodic functions with specific frequency and directions, instead of coordinates (or pixels) with intensity values. In analogy to microscopy, the FT works as a lens, and oppositely, a lens can be regarded as a Fourier transformer. There is a link to Lab1 exercise and the lecture block “imaging”.

Furthermore, FFTs are useful for image processing. Image processing with FFTs involves computing and modifying this FFT of an image, before computing the inverse FFT (IFFT).

This corresponds to mapping the image in the frequency domain (reciprocal space) and modifying this, before back-projecting the power spectrum into the spatial domain (real space). Image filtering is image processing where certain aspects of the image are emphasised. Masking is the simplest case, in which image intensities are thresholded based on their value or by their coordinates. Placing a mask in the frequency domain of an image, can be compared to placing an aperture in the diffraction pattern of an object studied in a microscope. For example, in a transmission electron microscope, different aperture positions in reciprocal space can be used to obtain bright-field or dark-field images formed by unscattered and scattered beam(s).
The information far out in reciprocal space corresponds to features in the image with small real-space periodicities, i.e. details in the input image (or object). An image can be noise-reduced by using a narrow mask, i.e. a low-pass filter, in reciprocal space. Noise-reduction competes with image blurring. One should be careful not to introduce artefacts or misinterpret images when performing such image/filtering processing.

Lab tasks
Your task is, starting from code provided, to demonstrate understanding and visualize 1) diffraction from different structures and 2) use image processing based FFTs/IFFTs. Be creative and play with different structural parameters for the given models. Be alert what actual is computed and plotted. This lab exercise should help understanding the main course concepts.

Part 1. Diffraction from one-dimensional crystals (Aim: link $\rho(x)$ and $I(q)$)
Illustrate and explain the differences between the following models and especially their corresponding simulated diffraction patterns; i) monoatomic basis, ii) diatomic basis, iii) disordered material (glass) and iv) material with thermal motion. You need to show both real and reciprocal, discuss the intensity distributions in reciprocal space and relate them back to charge densities in real space for structural parameters you investigated.

Part 2. FFTs and imaging (Aim: link diffraction and imaging)
By using your own images and/or the provided example images, illustrate and explain
(i) the appearance of the simulated diffraction patterns of differently shaped objects (e.g. triangles, squares, circles and periodic structures, own figures/phots),
(ii) image filtering, noise-reduction and blurring by masking certain parts of frequency space and generating inverse fourier transform (IFT).

Part 3. Diffraction from two-dimensional crystals
Illustrate and explain i) the differences between the simulated 2D diffraction patterns for the given model structures as done for 1D (part 1) and ii) make use of image processing tools introduced in part 2.

For the report part 1 and 3 are most essential. The code has comments and tips included. For the report have a writing plan. Report is submitted via a BB assignment, as group of max. 2.

Recommended literature:

[1] Aubert, E. & Lecomte, C. Illustrated Fourier transforms for crystallography. Journal of Applied Crystallography 40, 1153–1165 (2007).
URL http://journals.iucr.org/j/issues/2007/06/00/kk5014/kk5014.pdf.

[2] Pyhon code (notebook) at https://tinyurl.com/TFY4255-2024-lab2 or https://github.com/HelvoortTon/TFY4255_2024_Lab2