
Neutron and X-ray Scattering of Quantum Materials

PHYS-640

Week 2 exercises

1: The monochromator

- (a) Exercise 9.P.1 in the neutron notes.
- (b) Sometimes Si (111) is chosen instead of PG (002) for monochromating the neutron beam. Calculate the structure factor for the Si (nnn) reflections for $n = 1, 2, 3, 4$.
- (c) Can you think of why Si (111) is sometimes a better choice for the monochromator?

2: The crystal structure of Po and NaCl

- (a) Calculate the structure factor for Po and NaCl.
- (b) What is the main difference between the two examples?
- (c) Index the powder diffraction pattern of NaCl in Fig. 1.

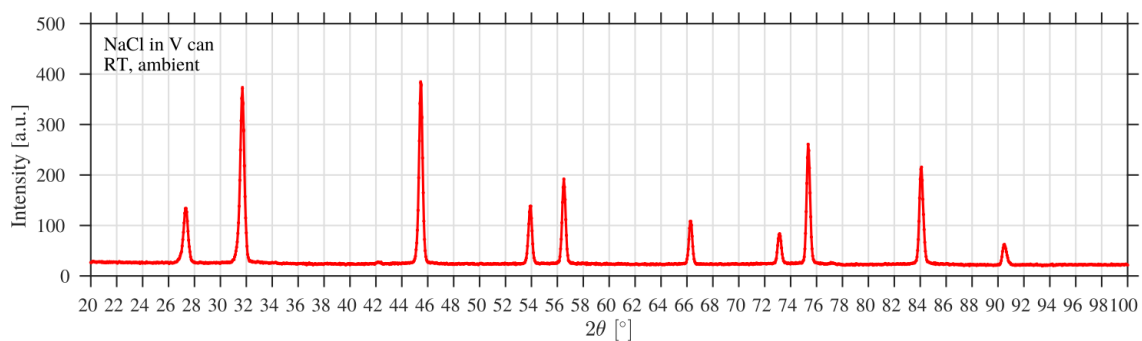


Figure 1: Neutron powder diffraction pattern on NaCl measured at room temperature (RT) and ambient pressure on the D20 diffractometer at the ILL. The wavelength used was $\lambda = 1.54 \text{ \AA}$.

- (d) NaCl is sometimes used as a pressure gauge when doing neutron scattering experiments under pressure. Using the equation of state (EoS) published by Brown et al. (<https://doi.org/10.1063/1.371596>, also on moodle), what is the change in scattering angle, 2θ , of the first Bragg peak when applying 3 GPa of hydrostatic pressure?

3: Time-of-flight neutron Laue diffraction with LiFePO₄

- (a) Calculate the structure factor for LiFePO₄ (atomic positions are uploaded on moodle). You probably want to write a little script for this rather than doing it by hand. Which are suitable Bragg peaks to use for aligning the sample in the (b, c)-plane?

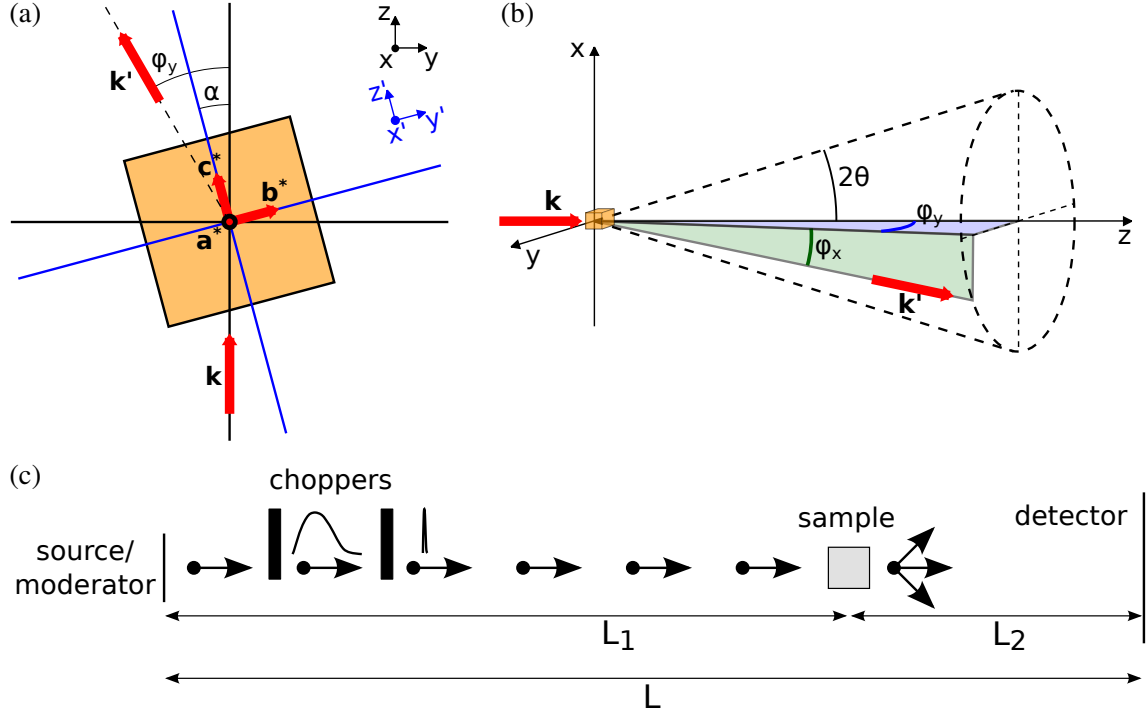


Figure 2: (a) Scattering geometry of the time-of-flight Laue diffraction experiment. The crystal is rotated an angle α with respect to the incoming beam. The scattered neutrons have a scattering angle φ_y with respect the z -axis. (b) The Debye cone with opening angle 4θ . The angle of the scattered neutrons with respect to the horizontal plane is φ_x . (c) Overall setup at NOBORU for time-of-flight neutron diffraction.

(b) Assume a $(\uparrow\uparrow\downarrow\downarrow)$ arrangement of spins in the unit cell. Is this structure commensurate or incommensurate? Which Bragg peak positions are suitable to look for this magnetic structure?

(c) In a time-of-flight Laue diffraction experiment performed on the NOBORU instrument at J-PARC, the single crystalline sample is oriented as shown in Fig. 2(a)-(b). Show that Bragg reflections in the $(0K0)$ direction scatter with the angle 2α in the horizontal plane

(d) The distance from the source to the sample is $L_1 = 14$ m and from the sample to the detector is $L_2 = 1.5$ m, see Fig. 2(c), and the rotation of the crystal was $\alpha = 7^\circ$. What is the flight times for the nuclear Bragg reflection (020) and the magnetic Bragg reflection (010) ?