X_ray

February 19, 2023

1 X-Ray Diffraction

```
[]: import numpy as np
import matplotlib.pyplot as plt
import scipy as sp
import scipy.optimize as opt
import scipy.constants as const

title_size = 20
axis_size = 16
```

1.1 Pre-lab Questions

- 1.a) Read labscript and relevant course material. Elements used from mathematical techniques are: scipy curve_fit and chi squared test.
- 1.b) From the equation $m\lambda = 2d\sin\theta$ from this for a higher wavelength the angle of diffraction will be greater than for a lower wavelength. As the energy of the K-alpha is lower as it comes from the n=2 to the n=1 shell, the wavelength will be higher and the angle of diffraction will be greater than that of the K-beta which comes from the n=3 to the n=1 shell.
- 1.c) Calculate the Interatomic spacing of a LiF cubic crystal using $d = \frac{a}{\sqrt{3}}$ where a is the lattice constant. First calculate the lattice constant from the mass and the density of the crystal.

$$\begin{split} \rho &= 2.64g/cm^3 \\ m_{tot} &= 25.94u \\ m_{tot} &= \frac{25.94}{6.022 \times 10^{23}} = 4.308 \times 10^{-23}g \\ Volume &= \frac{m_{tot}}{\rho} = \frac{4.308 \times 10^{-23}}{2.64} = 1.632 \times 10^{-23}cm^3 \\ a &= \sqrt[3]{Volume} = \sqrt[3]{1.632 \times 10^{-23}} = 2.536 \times 10^{-8}cm \\ d &= \frac{a}{\sqrt{3}} = \frac{2.536 \times 10^{-8}}{\sqrt{3}} = 1.46 \times 10^{-8}cm \end{split}$$