

Problem Set 3

Due date: June 23, 2017

1. (a) Simulate the $\theta - 2\theta$ powder diffraction pattern of sodium chloride at room temperature in the 2θ range between 20° to 80° . The average grain size in the sample is 50 nm. Cu $K\alpha$ radiation is used in the analysis. You should consider the structure factor, Lorentz-polarization factor, multiplicity, temperature effect, but ignore the background intensity due to temperature diffuse scattering.

(b) Using the software CaRINE to plot the X-ray powder diffraction pattern of sodium chloride.