Advanced Construction Materials

Homework #2

Due: April 9th at 6 pm

1. The sodium chloride structure has an FCC bravais lattice with cube side ***a***, and a two atom basis. The basis consists of a positively charged ion (Na^+) at origin and a negatively charged ion (Cl^-) at $\boldsymbol{(a/2)\vec{x}}$. If atomic form factor $f_- = f_+$, calculate structure factor and provide some examples (h,k,l) of diffraction peaks only for constructive interference. Also provide several examples (h,k,l) of vanished peaks. **(30pt)**

2. Using Mercury software, draw plots of X-ray diffraction of portlandite ($Ca(OH)_2$, COD ID#1001768) in different units of 1) *2theta* (from Cu k-alpha X-ray, λ=1.54056 Å), 2) *d-space*, and 3) *q-space*. **(20pt)**

3. In problem #2, we have three X-ray diffraction patterns in different units of *2theta*, *d-space*, and *q-space*. If you used a different source of X-ray (Molybdenum, λ=0.7107 Å), will any of these patterns be changed? Then draw the changed plot. **(20pt)**

4. Calcium sulfoaluminate (CSA) cement is one of sustainable cements being developed with less carbon footprint. Attachment contains data of X-ray diffraction pattern obtained from hydrated CSA cement at 1 day using Cu k-alpha X-ray, λ=1.54056 Å. Try quantitative phase analysis (QPA) to determine relative weight percentage of below three phases. From your refinement result, calculate R-indices of R_F. **(30pt)**

   Ye'elimite (COD ID#4001772)

   Gypsum (COD ID#1010981)

   Ettringite (COD ID#1520837)