XRD 1

Session 1: 56 pts

1. Significance of Start angle = 20° **1 pt**

2. Standard deviation analysis (for Cu only) **3 pts**

3. Calculation of Structure factors for HCP, Diamond and ZnS crystal structures **12 pts (4 pts for each material)**

3. Table listing allowed diffractions (hkl), d, $2\theta_{calc,}$ $2\theta_{expt}$ and $2\theta_{error}$ for Cu, Mo, Ti, Si and ZnS **25 pts (5 pts for each material)**

4. Intensity vs 2θ plot on Matlab **15 pts (3 pts for each material)**

Session 2: 44 pts

6. Lattice constant error analysis:
   a) Calculation of lattice const corresponding to the 4 tallest peaks for Cu, Mo and Si **6 pts (2 pt for each cubic material)**
   b) a vs 2θ plot at different scan speeds and calculation of uncertainty in a for Cu **3 pts**
   c) Discussion on the relationship between scan speed and uncertainty in a **4 pts**
   d) Determination of lattice constant by extrapolation of a vs $\cos^2\theta/\sin\theta$ plot for Cu, Mo and Si using Matlab **6 pts (2 pt for each cubic material)**
   e) Discussion on the relative magnitudes of systematic and statistical errors and their implications **4 pts**

7. Characterization of Cu-K_α doublet
   a) Determination of λ_1/λ_2 experiments and comparison with theoretical ratio **4 pts**
   b) Explanation of the presence of doublet peaks **3 pts**
   c) Estimation of intensity ratio of the two Cu-K_α lines **3 pts**

8. Structure factor analysis
   a) Explanation of differences between Cu, Si and ZnS spectra **6 pts**
   b) Estimation of $\dfrac{\left|f_A + f_B\right|^2}{\left|f_A - f_B\right|^2}$ for ZnS and calculation of $\dfrac{f_A}{f_B}$ **5 pts**