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, 2θ<sub>calc</sub>, 2θ<sub>expt</sub> and 2θ<sub>error</sub> 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 cos²θ/sinθ 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-Kα doublet
   a) Determination of λ<sub>1</sub>/λ<sub>2</sub> 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-Kα lines 3 pts

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