**Introduction to Crystallography**

**Final Examination, December 13th, 2008**

**Name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_, Student ID.: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

**Total 370 points (40%), 18:00 ~ 21:00 (3 hours)**

1. Briefly explain the following terms. Choose 20 questions out of 22. You will get *penalties* for choosing more than 20.

(Total 100 points, 5 each)

(1) Zonal equation

(2) Primitive translation vector

(3) Crystal structure

(4) Wurzite crystal structure

(5) Sapphire crystal structure

(6) Wulff net

(7) Compound symmetry operations

(8) Euler's construction

(9) Crystal system

(10) Bravais lattice

(11) Schonflies notation

(12) Neumann's principle

(13) Diffraction

(14) Amplitude function

(15) Fourier transformation

(16) Convolution

(17) Reciprocal lattice

(18) Structure factor

(19) Laue condition

(20) Bragg's Law

(21) Ewald sphere

(22) Powder diffraction

(in relation to the Ewald sphere construction and the reciprocal lattice)

1. (a) When you have a slit with a width of A and height of 1/A, centered at x=0, show how the intensity of the wave diffracted from this slit varies with sinθ.

(b) If the width of the slit is decreased down to 0, which results in a delta function, how would the diffracted-wave intensity vary with sinθ.

(20 points)

1. Assume N-narrow slits (N δ-functions) equally spaced by a distance of x0. Let the number of slits be N = 2p+1. Derive the wave function, F(sinθ), of the diffracted wave step-by-step. Then, expand this equation to the case of a 3-D array of narrow slits, which represents a lattice with unit vectors of , , and . Explain how this leads to the construction of the reciprocal lattice. (You don’t have derive the actual reciprocal unit vectors, just explain how it should be done)

(30 points)

1. During the class, it has been shown that the Laue condition and Bragg's Law are basically identical. Show this by deriving the Bragg’s Law from the Laue condition.

(20 points)

1. Draw the following structures and write down the structure factor of each. Identify the reciprocal lattice points indicating the relative intensity of each point. Now, if you are using an X-ray with λ = 0.143 nm to identify the structure of each crystals, write down the scattering angles 2θhkl of the first five peaks with different scattering angles. (i.e. five lowest angles) Remember that λ =2dhkl·sinθ.

(100 points)

(a) FCC structure

(b) HCP structure

(c) CsCl structure

(d) CaF2 structure

(e) NaCl structure

\* Assume a=5Å for (a),(c),(d),(e) and atomic radius = 2.5Å with an ideal c/a ratio for (b).

1. Consider the trigonal prismatic interstice (i.e. formed by an equi-triangular array of three atoms placed directly above an identical group of three atoms). What is the interstice atom to host atom size ratio? Notice that this is not an octahedral interstice even though the coordination number is six.

(30 points)

1. The WC structure can be described as consisting of closed-packed planes of W atoms, stacked directly on top of one another, with C occupying half of the trigonal prismatic interstices forming an identical array to that of the W atoms.

(70 points)

1. Based on this description, draw the unit cell of WC and give its axial ratio (assuming isotropic metallic bonding).
2. If rC=0.75 Å and rW=1.37 Å, do the metal atoms contact each other?
3. What is the stacking sequence?
4. What is the Miller index of the shortest vector from a W atom to a C atom?
5. What is the length of this vector?
6. What is the point symmetry at a W atom?
7. Derive the structure factor for 0001, 0002, 100 reflections. (in diffraction)