

**ASSIGNMENT 3**

Problems: due Monday, September 22, 2003.

1. In the fcc lattice extra atoms may be introduced into “tetrahedral” and “octahedral” sites—the surrounding lattice atoms lie at the vertices of a regular tetrahedron or octahedron. Determine where the interstitial sites are located.

2. In a Debye-Scherrer diffraction experiment, the Bragg angles are found using Cu  $K_{\alpha}$  radiation. The sample is granular Al, which has atomic weight 27 and density  $2.7 \text{ g cm}^{-3}$ . Calculate Avogadro’s number given the following diffraction angles (in deg).

19.48	41.83
22.64	50.35
33.00	57.05
39.68	59.42

3. KCl and KBr are alkali halides with the NaCl structure. The table lists the X-ray reflections observed (and absent) from low-index planes. Why is there a difference between two similar crystallographic structures? Be as quantitative as possible.

<b>KBr</b>	(111)	(200)	(220)	(311)	(222)	(400)	(331)	(420)
<b>KCl</b>		(200)	(220)		(222)	(400)		(420)

4. In highly symmetrical structures, many families of planes are equivalent and possess the same interplanar spacing; these planes therefore contribute to the same equivalent diffraction line. In cubic systems the planes (123), (321), (213) are equivalent planes but not for orthorhombic systems. The total number of equivalent planes for a given  $hkl$  is called the *multiplicity*. It, along with the structure factor, influences the intensities of diffraction lines. Taking into account positive and negative values of the  $hkl$ , calculate the multiplicities of the following types of planes in both cubic and orthorhombic structures:  $(hkl)$ ,  $(hhl)$ ,  $(hhh)$ ,  $(0kl)$ ,  $(0kk)$ , and  $(00l)$ .

5. Si and GaAs have the same crystal structure which is represented by a fcc lattice with a basis. The bases are (in units of the cubic lattice parameter), for Si: Si (000) and Si ( $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ ); for GaAs, Ga(000) and As( $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ ). Determine the Miller indices of the allowed Debye-Scherrer reflections for these semiconductors.