HW Number 3

1) NiAl has a cubic structure with a=b=c=2.888 Angstroms with, in the ordered phase, Ni at (0,0,0) and Al at (0.5,0.5,0.5). The disordered phase has an equal fraction (statistically) or Ni and Al at each site. Using fAu and fCu to represent the atomic electron scattering factors, derive the general form of the structure factors as a function of (hkl) for both the ordered and disordered phases.

2) Silicon has the "diamond" fcc structure with a lattice parameter of 0.543nm, and along a [111] direction has an AABBCCAABBCC... stacking.

 a) What are the allowed diffraction spots for silicon?

b) For a [111] orientation, what will be the general form of the diffraction pattern (be careful to consider what spots are allowed and what are not)?

 c) A simplified method of taking account of the effects of covalent bonding is to consider Gaussian features of additional charge density half-way between the atoms, e.g. C. Scheringer, *Acta Cryst.* (1980). A36, 205-210. Show that whereas the (222) reciprocal lattice spot has zero intensity with just the atomic scattering factors, it becomes non-zero when the midpoint features modelling bonding are included.

3) For a bcc material, a diffraction pattern taken along [001], all the diffraction spots show streaks running along (100) and (010). Using only transmission electron diffraction, design a set of experiments to determine what these are due to in real space. Hint: be careful and systematic, otherwise you will never get anywhere.