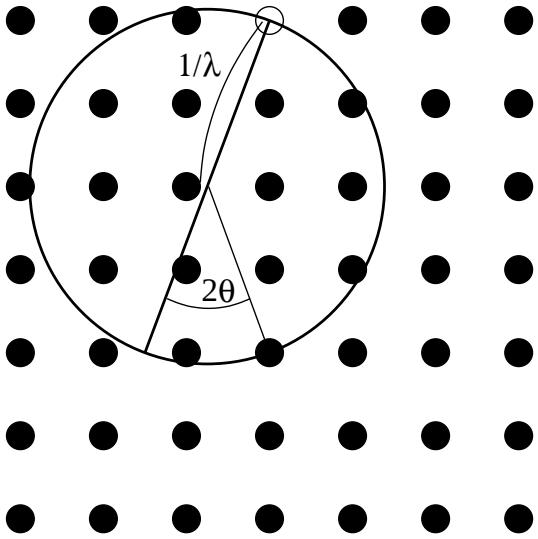
B6, 1999

1 Ewald sphere

The Ewald sphere construction is a geometrical operation applied to a reciprocal lattice in order to explore the diffraction characteristics exhibited by a crystal when a probing beam with a given wavelength is incident at a given orientation. The sphere, which has a radius $1/\lambda$ is oriented such that a diameter lies parallel to the incident beam, with one end of this diameter fixed at the origin of reciprocal space.



The Bragg condition is satisfied for any reciprocal lattice point lying on the surface of the Ewald sphere. This can be seen by considering the right-angled triangle with the sphere diameter as hypothenuse.

The Ewald sphere construction is applicable for any probing beam. It is most commonly applied to X-Rays and electron beams. However, it may be noted that these typically have very different wavelengths:

	X-rays	Electrons
λ	$\sim$0.1 nm	$\sim$0.003 nm
$1/\lambda$	10 nm^{-1}	300 nm^{-1}

Thus, while the diameter of the Ewald sphere is of same order as d_{hkl} for x-rays, it is much greater for an electron beam. Furthermore, since electrons only penetrate short distances through most crystals, specimen are normally thin, which has the effect of elongating the reciprocal lattice spots parallel to

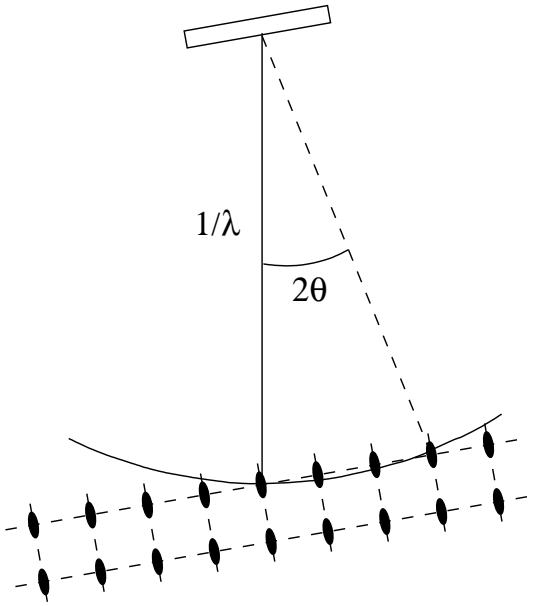


Figure 1: Ewald sphere for electron diffraction.

the beam direction. Thus, for electron diffraction, the ES construction looks something like figure 1 so that a monochromatic beam gives a diffraction pattern approximating to a plane of the reciprocal lattice.

2 Systematic absences

Systematic absences arise with non-primitive lattices, as a consequence of reflections from arrays of atomic planes which destructively interfere with primitive reflections. For example, consider 100 reflections:

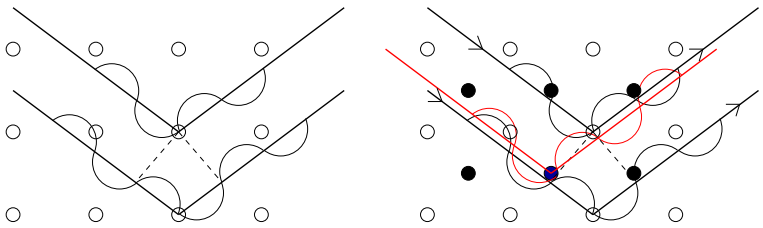
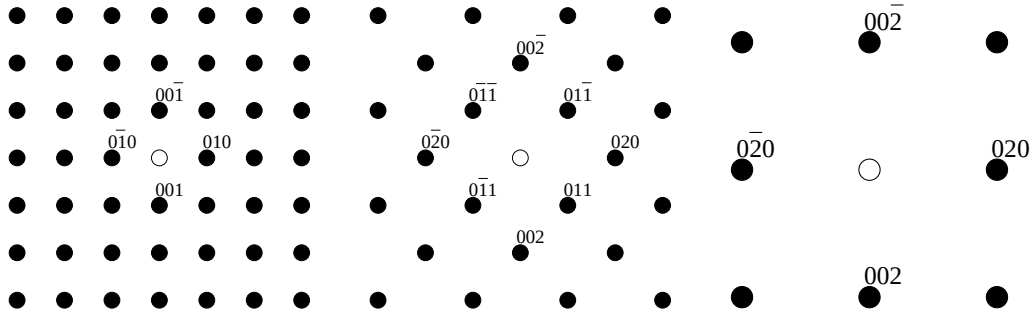


Figure 2: Left: (100) reflection in a P lattice. Right: this reflection is absent in an F lattice.

Reciprocal lattice sections:



3 Diffractometer traces for Cu3Au

The high-temperature form appears to have an F lattice, while the low temperature one has a P lattice. This is explained if we note that, at high temperature, the solution is disordered, and there is a probability of 25% to find Au / 75% to find Cu on each points of a F lattice. At low temperature, the Au atoms occupy the corner of the cube while the Cu occupy the centre of the faces (and therefore 3 Cu for 1 Au)

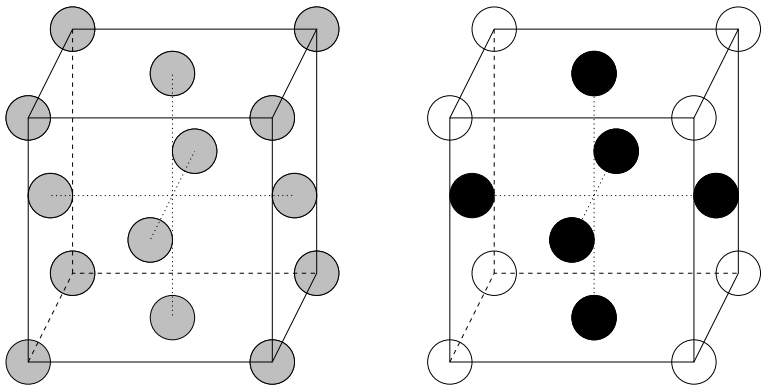


Figure 3: Left: disordered state, Cu and Au have 75% and 25% (resp.) probability to occupy any lattice point. The lattice is F. Right: ordered state, the lattice is P

4 Peak height variations:

- geometric effect: the diffractometer will normally sample a lower proportion of the total diffracted beam for higher reflection angles (as-

suming the diffractometer samples a fixed solid angle subtended at the specimen). Higher angle reflections therefore have lower intensities.

- Multiplicity: some planes have more equivalent sets than others, and since each equivalent set will tend to contribute equally to the intensity, reflections with higher multiplicity will be stronger than those with lower multiplicities.

- Each reflection has a characteristic structure factor, which is an indication of the number of atoms per unit cell which lie in the planes concerned and the efficiency with which the atoms concerned scatter X-rays (scattering factors of the atom).

A geometric effect is apparent (trend for higher angle reflections to be of lower intensity). Multiplicity can account for some effects (e.g. 111 has multiplicity 8 compared to 6 for 100) but seems to have a weak influence here. The structure factor accounts for the remaining effects, planes such has 111 have a lot of atoms, other rather few. Note that Au is a stronger scatterer than Cu.