Lattice Planes and Miller Indices

A lattice plane (or crystal plane) is a plane contain- ing at least three non-collinear (and therefore an infinite number of) points of a lattice. A family of lattice planes is an infinite set of equally separated parallel lattice planes which taken together contain all points of the lattice.

The orientation of a crystal plane is determined by three points in the plane, provided they are not collinear. If each point lay on a different crystal axis, the plane could be specified by giving the coordinates of the points in terms of the lattice constants a, b, c. However, it turns out to be more useful for structure analysis to specify the orientation of a plane by the indices determined by the following rules

- Find the intercepts on the axes in terms of the lattice constants a, b, c. The axes may be those of a primitive or nonprimitive cell.
- Take the reciprocals of these numbers and then reduce to three integers having the same ratio, usually the smallest three integers. The result, enclosed in parentheses (hkl), is called the index of the plane.

For the plane whose intercepts are $4, 1, 2$, the reciprocals are $\frac{1}{4}$, 1, and $\frac{1}{2}$ the smallest three integers having the same ratio are (142). For an intercept at infinity, the corresponding index is zero. The indices of some important planes in a cubic crystal are illustrated by Fig. The indices (hkl) may denote a single plane or a set of parallel planes. If a plane cuts an axis on the negative side of the origin, the corresponding index is negative, indicated by placing a minus sign above the index: $(h\bar{k}l)$.

The interplanar distance between two successive plane of indices (h, k, l) in an orthogonal lattice is given by,

$$d = \frac{1}{\left(\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right)^{1/2}}$$

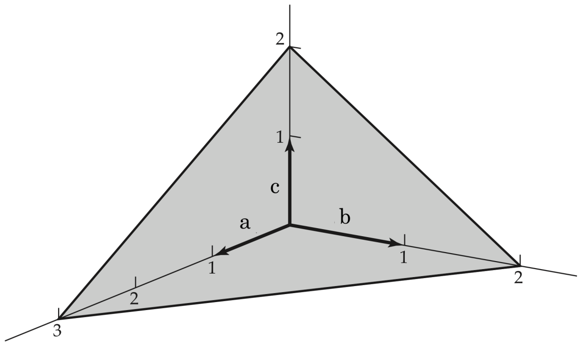

Figure 1: This plane intercepts the a, b, c axes at $3a$, $2b$, $2c$. The reciprocals of these numbers are $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$. The smallest three integers having the same ratio are $2, 3, 3$, and thus the indices of the plane are (233).

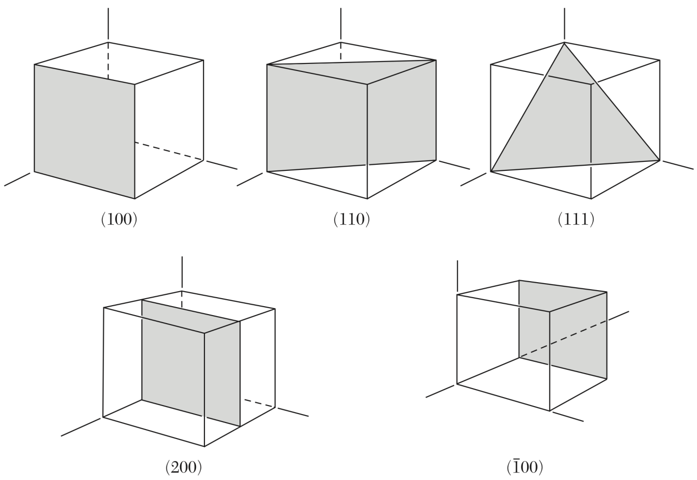

Figure 2: Indices of important planes in a cubic crystal. The plane (200) is parallel to (100) and to ($\bar{1}$00).

Diffraction of Waves by Crystals

The Bragg law We study crystal structure through the diffraction of photons, neutrons, and electrons . The diffraction depends on the crystal structure and on the wavelength. At optical wavelengths such as 5000Å, the superposition of the waves scattered elastically by the individual atoms of a crystal results in ordinary optical refraction. When the wavelength of the radiation is comparable with or smaller than the lattice constant, we may find diffracted beams in directions quite different from the incident direction.

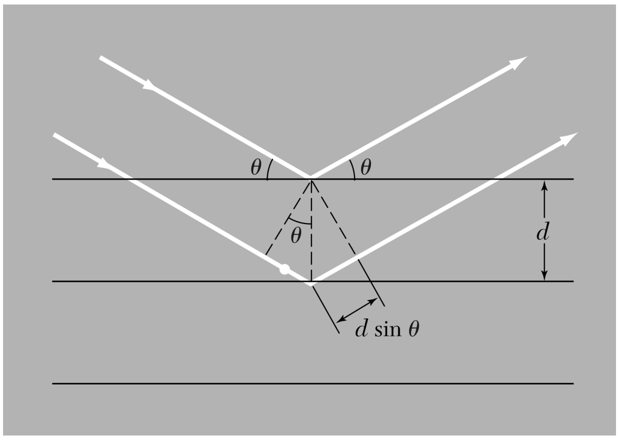

Figure 3: Bragg Law.

W. L. Bragg presented a simple explanation of the diffracted beams from a crystal. The Bragg derivation is simple but reproduces the correct result. Suppose that the incident waves are reflected from parallel planes of atoms in the crystal, with each plane reflecting only a very small fraction of the radiation, like a lightly silvered mirror. In specular (mirrorlike) reflection the angle of incidence is equal to the angle of reflection. The diffracted beams are found when the reflections from parallel planes of atoms interfere constructively. We treat elastic scattering, in which the energy of the x-ray is not changed on reflection.

Consider parallel lattice planes spaced d apart. The radiation is incident in the plane of the paper. The path difference for rays reflected from adjacent planes is $2d \sin\theta$, where θ is measured from the plane. Constructive interference of the radiation from successive planes occurs when the path difference is an integral number n of wavelengths λ, so that

$$2d \sin\theta = n\lambda$$

This is the Bragg law, which can be satisfied only for wavelength $\lambda \leq 2d$.

Although the reflection from each plane is specular, for only certain values of θ will the reflections from all periodic parallel planes add up in phase to give a strong reflected beam. If each plane were perfectly reflecting, only the first plane of a parallel set would see the radiation, and any wavelength would be re- flected. But each plane reflects 10^{-3} to 10^{-5} of the incident radiation, so that 10^3 to 10^5 planes may contribute to the formation of the Bragg-reflected beam in a perfect crystal.

The Bragg law is a consequence of the periodicity of the lattice. Notice that the law does not refer to the composition of the basis of atoms associated with every lattice point. We shall see, however, that the composition of the basis determines the relative intensity of the various orders of diffraction (denoted by n above) from a given set of parallel planes.