Reciprocal Space and x-ray diffraction

Due to 3D the periodic arrangement of atoms (molecules) in a crystal one can find "dense packed planes" = **lattice planes**, in certain directions of space. Assuming one of these lattice planes makes an intersection point with the a, b, c axes with the ratios $ma; nb; pc$,~~-~~defining the direction of the normal of this plane by $\vec{r} = ma\ + nb\ + pc$ the inverse ratio normalized to integer values $\frac{1}{m};\frac{1}{n};\frac{1}{p} = h,k,l$ define the **Miller indices** h,k,l which are integer multiples of a vector ***k*** in reciprocal space $\vec{k} = ha^* + kb^* + lc^*$. Miller indic~~e~~es of the main plane cutting the a-axis of a cube are (100), its normal vector is [100]. The shortest distance between two neighboured lattice planes is the **lattice plane distance d**; d is a function of h,k,l and the lattice parameters. In cubic system it is given by $d = \frac{a}{\sqrt{h^2+k^2+l^2}}$ ~~-~~; in hexagonal system it is

$$d = \frac{a}{\sqrt{\frac{4}{3}(h^2+k^2+hk)+\frac{a^2}{c^2}l^2}};$$

The reciprocal lattice is related to the periodicity of the crystal lattice and can be considered as it's Fourier-transformation. The basis vectors $\mathbf{b}_i$ of the reciprocal lattice are related to the basis vectors $\mathbf{a}_i$ by the relation

$$\mathbf{b}_i = 2\pi\,\varepsilon_{ijk}\frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}$$ and fulfill the relation $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\,\delta_{ij}$.

In crystal systems with 90° angles between axes b_i^* is parallel to a_i and reciprocal in length $b_i^* = 2\pi/a_i$. Because the wave length of x-rays are in same order of magnitude as lattice spacing a, the arrangement of atoms in a crystal can be studied by an x-ray diffraction experiment. The interference condition of a x-ray wave with a 3D crystal has been derived by Max v.Laue in 1912. If $\alpha_0,\beta_0,\gamma_0$ are the angles of incidence and $\alpha\ ,\beta\ ,\gamma$ the angles of exit with respect to the axes a,b,c one can find 3 conditions to be fulfilled simultaneously in order to obtain a diffraction maximum in 3D space: Maxima appear whenever:

$g_x(\cos\alpha - \cos\alpha_0) = \pm h\,\lambda$; $g_y(\cos\beta - \cos\beta_0) = \pm k\lambda$; $g_z(\cos\gamma - \cos\gamma_0) = \pm l\,\lambda$

For a certain set of Miller indices *h,k,l* this is possible only for a single wave length.

$$\boxed{\lambda = \frac{2\frac{N_z}{g_z}}{(\frac{N_x}{g_x})^2+(\frac{N_y}{g_y})^2+(\frac{N_z}{g_z})^2}}$$ Laue´s interference condition

An alternative relation to obtain an interference maximum has been derived by Bragg: **N λ = 2d sin Θ**, where Θ is the reflection angle with respect to a set of lattice planes with spacing d. A graphic tool to solve Laue´s and Bragg´s equations is the concept of Ewald´s sphere.

The Intensities of the Bragg reflections (see Laue Interference) depend on the number of unit cells within the crystal (shape factor, S) $\boxed{S = \frac{\sin^2(N\frac{\pi d}{\lambda}\sin\alpha)}{\sin^2(\frac{\pi d}{\lambda}\sin\alpha)^2}}$ and the relative coordinates of atoms within the unit cell structure factors $F = \sum_n f_n \exp(-2\pi i(hx_i + ky_i + lz_i))$. The scattering intensity is proportional to S² and F². Typical diffraction experiments executed in Siegen´s Lab. practicum) are the Laue diffraction and Debye-Scherrer-Experiment. The Solid State Physics representation of a primitive reciprocal unit cell is the Brillion zone.