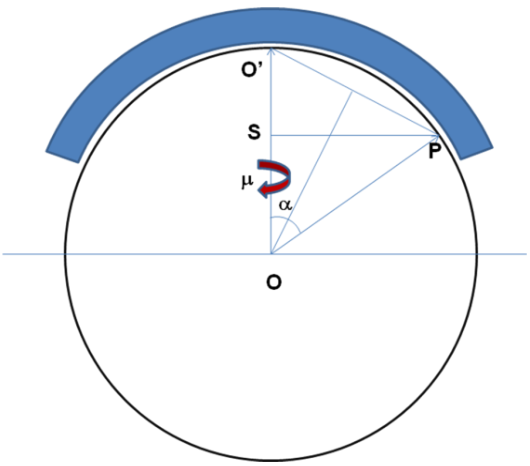
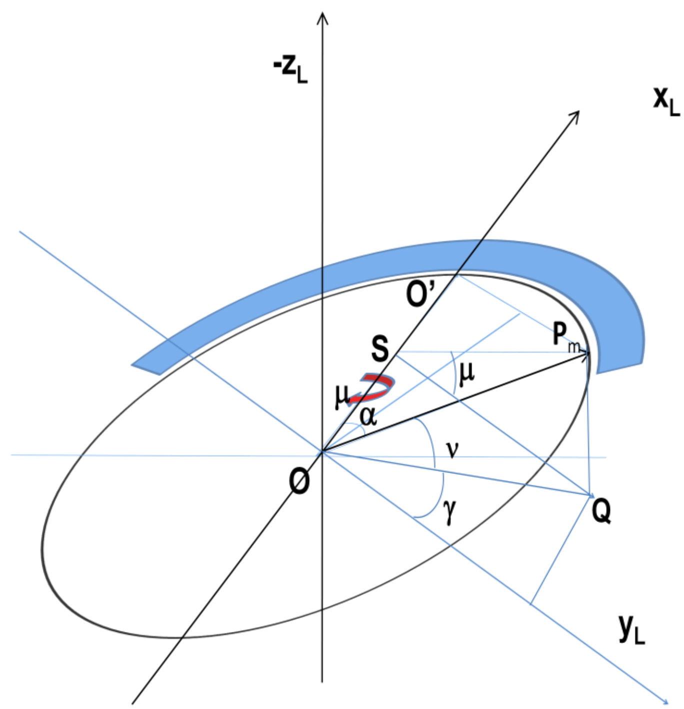
Flat-cone geometry in D10 (J. Rodríguez-Carvajal)

The banana detector of radius R is supposed to be fixed to the arm along the $\mathbf{x}_L$ axis and has the possibility to be rotated by an angle μ around $\mathbf{x}_D=\mathbf{x}_L$. We defined a detector frame having the same orientation as the laboratory system when μ=0. Notice that for D10 we use a Busing-Levy L-system with the $\mathbf{z}_L$-axis pointing downwards. For a general position of the detector the relation between the L and D systems is given by the matrix providing the components of a vector in the D system when their components in L are known:

$$\mathbf{v}_D = \mathbf{M}\cdot\mathbf{v}_L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\mu & \sin\mu \\ 0 & -\sin\mu & \cos\mu \end{bmatrix}\cdot\begin{pmatrix} v_{1L} \\ v_{2L} \\ v_{3L} \end{pmatrix}$$

A diffracted beam impinging the detector is shown in the following figure. We can deduce the relations between the angles (μ, α) of the detector and the angles (γ, ν) of the diffracted beam from the geometry shown in the figure.





From the figure on the left side one can see that:

$$OO'=OP=R, \quad OS = R\cos\alpha, \;\; SP = R\sin\alpha.$$

So, in the detector system the vector **OP** is **OP** = (R$\cos\alpha$, R $\sin\alpha$, 0), when the detector is rotated an angle μ the vector moves as shown on the right figure, so **OP** becomes **OP**$_m$.

We have the relations: $\mathbf{OP}_m$ = $\mathbf{M}$ $\mathbf{OP}$, and, on the other hand the vector $\mathbf{OP}_m$ has the following components with respect to the L-system $\mathbf{OP}_m$= R ($\cos\nu \sin\gamma$, $\cos\nu \cos\gamma$, $\sin\nu$), so we have the following relation

$$\mathbf{OP}_m = \mathbf{M}\cdot\mathbf{OP} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\mu & \sin\mu \\ 0 & -\sin\mu & \cos\mu \end{bmatrix} \cdot \begin{pmatrix} \cos\alpha \\ \sin\alpha \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\nu\sin\gamma \\ \cos\nu\cos\gamma \\ \sin\nu \end{pmatrix}$$

In which we have dropped the common factor R. Doing that we have the relations between the unitary vectors of the diffracted beam in both the L and D system

$$\mathbf{s}_{1L} = (\cos\nu\sin\gamma, \cos\nu\cos\gamma, \sin\nu)$$

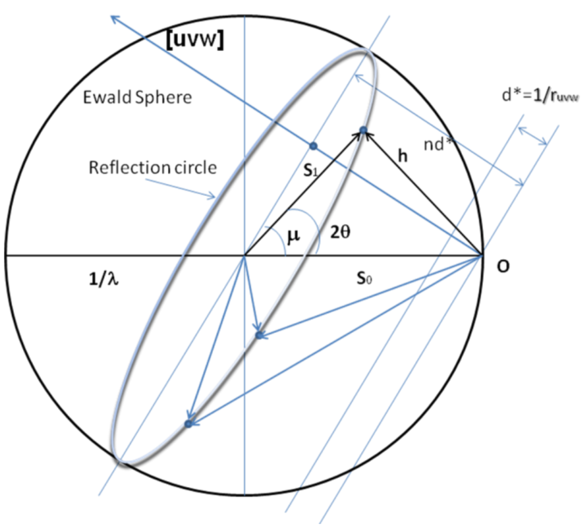
$$\mathbf{s}_{1D} = (\cos\alpha, \sin\alpha, 0)$$

The relations between the angles (μ, α) of the detector and the angles (γ, ν) of the diffracted beam can be deduced from the equations above, so that:

$$\cos\alpha = \cos\nu\sin\gamma; \quad \cos\mu\sin\alpha = \cos\nu\cos\gamma; \quad -\sin\mu\sin\alpha = \sin\nu$$

$$\sin\nu = -\sin\mu\sin\alpha \qquad \tan\gamma = \frac{\cos\alpha}{\cos\mu\sin\alpha}$$

The flat cone geometry allows the measurement of a reciprocal plane by rotating the crystal around a direct zone axis. A direct zone axis $\mathbf{r}_{uvw}$=[uvw] has a series of perpendicular reciprocal planes with inter-planar spacing $d^*=1/|\mathbf{r}_{uvw}|$. The plane passing through the origin of the reciprocal space is called the zero-level plane (n=0), the parallel plane situated at the distance nd^* from this plane is called the n-level plane. By orienting the crystal in such a way as making the n-level plane pass through the centre of the Ewald sphere the reflection circle is a maximum circle making an angle μ with the incident beam.



The orientation angle is related to the inter-planar spacing and the wavelength by the relation:

$$\sin\mu = \frac{nd^*}{1/\lambda} = \lambda n d^* = \frac{\lambda n}{|\mathbf{r}_{uvw}|}$$

This angle can be calculated knowing the cell parameters the desired level (n) and the wavelength of the radiation. Rotating the detector by the same angle with respect to the $\mathbf{x}_L$ axis one can record the reflections lying in this plane by rotating the crystal around the zone axis [uvw]. In order to record this reciprocal plane in the detector, the direct vector $\mathbf{r}_{uvw}$ should be oriented perpendicularly to the detector plane. Let us call the unitary vector along [uvw], $\mathbf{n}_{uvw}$. This unitary vector should adopt the form $\mathbf{n}_D$=(0,0,1) at the desired orientation in the detector system. There is an infinite number of ways of choosing ϕ, χ

and ω so as to reach the desired orientation, knowing the **UB** matrix; the Cartesian components of $\mathbf{r}_{uvw}$ with respect to the laboratory system when all angles are zero (ϕ-system) can be obtained by the expression:

$$\mathbf{r}_L = \mathbf{UB}\cdot\mathbf{G}\cdot\mathbf{r}_{uvw} = \mathbf{UB}\cdot(\mathbf{UB})^{-1}\cdot((\mathbf{UB})^{-1})^T\cdot\mathbf{r}_{uvw} = ((\mathbf{UB})^{-1})^T\cdot\mathbf{r}_{uvw}$$

Where **G** is the metric tensor ($\mathbf{G}_{ij} = \mathbf{a}_i\cdot\mathbf{a}_j$) transforming a vector with components referred to the direct lattice to the same vector with components referred to the reciprocal lattice. The four-circle matrix $\mathbf{R} = \mathbf{\Omega}\ \mathbf{X}\ \mathbf{\Phi}$ (active rotations), allows to orient the vector $\mathbf{r}_1 = \mathbf{r}_L / |\mathbf{r}_L|$ to the desired position

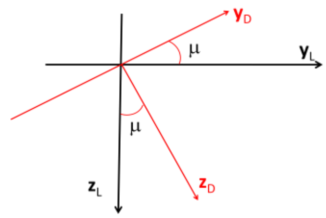
$$\mathbf{n}_4 = \mathbf{R}\cdot\mathbf{r}_1 = \mathbf{\Omega}\cdot\mathbf{X}\cdot\mathbf{\Phi}\cdot\mathbf{r}_1$$

Starting with the relation:

$$\mathbf{r}_L = ((\mathbf{UB})^{-1})^T\cdot\mathbf{r}_{uvw}$$

that gives the coordinates of the zone axis [*uvw*] in reciprocal space and with components in the Cartesian L-system when all angles of the orienting device are zero; we can calculate one of the orientation matrices that put the vector $\mathbf{r}_L$ in the direction of the vector normal to the flat-cone detector plane which is, in our case and with respect to the L-system, given by:

$$\mathbf{d}_L = \mathbf{z}_D = (0, \sin\mu, \cos\mu)$$



For that we use the cross product of $\mathbf{r}_1 = \mathbf{r}_L / |\mathbf{r}_L| = (a, b, c)$ (unitary vector along [*uvw*] in L-system) by $\mathbf{d}_L$. The result gives the axis of rotation needed to construct the rotation matrix. The angle between the two vectors can be obtained from the dot product.

$$\mathbf{n}=\mathbf{r}_1\times\mathbf{d}_L = \begin{vmatrix} \mathbf{x}_L & \mathbf{y}_L & \mathbf{z}_L \\ a & b & c \\ 0 & \sin\mu & \cos\mu \end{vmatrix} = (b\cos\mu - c\sin\mu)\mathbf{x}_L - a\cos\mu\,\mathbf{y}_L + a\sin\mu\,\mathbf{z}_L = (n_x, n_y, n_z)$$

$$\delta = \cos^{-1}(b\sin\mu + c\cos\mu)$$

The general expression of a rotation of angle ρ around the axis **n** in the L-system is provided by the Gibbs matrix in terms of the angle ρ and the director cosines of $\mathbf{n}=(n_x, n_y, n_z)$:

$$\mathbf{G}(\rho,\mathbf{n}) = \begin{bmatrix} \cos\rho + n_x^2(1-\cos\rho) & n_x n_y(1-\cos\rho) - n_z\sin\rho & n_x n_z(1-\cos\rho) + n_y\sin\rho \\ n_x n_y(1-\cos\rho) + n_z\sin\rho & \cos\rho + n_y^2(1-\cos\rho) & n_y n_z(1-\cos\rho) - n_x\sin\rho \\ n_x n_z(1-\cos\rho) - n_y\sin\rho & n_y n_z(1-\cos\rho) + n_x\sin\rho & \cos\rho + n_z^2(1-\cos\rho) \end{bmatrix}$$

In our case the matrix rotating the vector $\mathbf{r}_1$ (parallel to [*uvw*]) towards the normal to the detector plane, $\mathbf{d}_L$, is given by $\mathbf{G}(\delta, \mathbf{n})$, using the above expressions. This is just a particular rotation; there are an infinite number of rotations that place the vector $\mathbf{r}_1$ along the vector $\mathbf{d}_L$. A rotation matrix given by $\mathbf{R}= \mathbf{G}(\rho, \mathbf{d}_L)\ \mathbf{G}(\delta, \mathbf{n})$ applied to $\mathbf{r}_1$, with an arbitrary angle ρ, is also a solution. From the total rotation matrix, by varying ρ, we can get the Euler (ω, χ, ϕ) angles that rotates the crystal around $\mathbf{d}_L$ having first put the zone axis along this vector. The angles (ω, χ, ϕ) inside the available limits give the region of the reciprocal space that can be measured.

The calculations of the Euler (ω, χ, ϕ) to make an equivalent rotation matrix $\mathbf{R}(\omega, \chi, \phi)$ can be done by writing the equality:

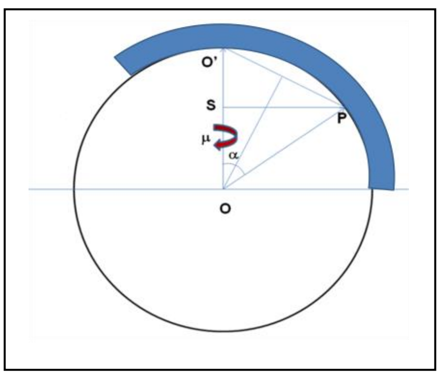
$$\mathbf{R} = \mathbf{R}(\omega,\chi,\phi) = \mathbf{\Omega}\cdot\mathbf{X}\cdot\mathbf{\Phi} = \mathbf{G}(\psi,\mathbf{d}_L)\mathbf{G}(\delta,\mathbf{n})$$

We can calculate the angles ϕ, χ and ω by the expressions:

$$\omega = ATAN2(-R_{23}, R_{13})$$
$$\chi = ATAN2(\sqrt{R_{31}^2 + R_{32}^2}, R_{33})$$
$$\phi = ATAN2(-R_{32}, -R_{31})$$

Calculation of the reciprocal points measured in the detector

The banana detector in D10 is asymmetric: the angular range has 30 degrees on the high angle side and 90 degrees on the low angle side with respect to the rotation μ-axis. Seen from the top the image of the detector appears as in the figure. If we call $\alpha(i)$ the α-angle corresponding to wire number i and we have N_w wires, we start numbering from 1 (lowest γ-angle) to N_w (highest γ-angle). In the case of D10 we have $\alpha(1) = 90°$ and $\alpha(N_w) = \alpha(128) = -30°$. The total angular range spanned by the banana detector is $\Delta=\alpha(1)-\alpha(N_w) = 120°$.



Once the angle μ has been set, the diffracted beam vectors corresponding to the different wires of the detector are fixed and obtained easily from (α,μ). The (γ,ν) angles are obtained using the equations:

$$\alpha(i) = \alpha(1) - (i-1)\frac{\alpha(1)-\alpha(N_w)}{N_w - 1}$$

$$\sin\nu(i) = -\sin\mu\sin\alpha(i) \qquad \tan\gamma(i) = \frac{\cos\alpha(i)}{\cos\mu\sin\alpha(i)}$$

The α-angle is always in the interval [-30°, 90°] for D10. The scattering vectors for each pixel are obtained in the L-system from the (γ, ν) angles and the wavelength as:

$$\mathbf{z}_4(i) = \frac{\mathbf{s}_{1L}(i) - \mathbf{s}_{0L}}{\lambda} = \frac{1}{\lambda}[\cos\nu(i)\sin\gamma(i),\ \cos\nu(i)\cos\gamma(i) - 1,\ \sin\nu(i)]$$

The reciprocal lattice coordinates of the scattering vectors are obtained from the setting angles (ω, χ, ϕ) and the UB-matrix as:

$$\mathbf{z}_4(i) = \Omega\mathrm{X}\Phi UB\mathbf{h}(i) \qquad \leftrightarrow \qquad \mathbf{h}(i) = (UB)^{-1}\Phi^T\mathrm{X}^T\Omega^T\mathbf{z}_4(i)$$