Previous: Introduction
Next: Computer systems

NONIUS CAD4/MACH3
User manual

21 December 2000

CAD4 geometry

Definitions
Mechanical alignment
Rotation about an axis in the coordinate system X,Y,Z
Rotation of a sample in the CAD4 geometry
Setting a reflection
Transformation from Miller indices to kappa geometry
Transformation from kappa geometry to Miller indices

Definitions

The geometry of the CAD4 differs from the geometry of the "classical" Eulerian cradle four- circle diffractometer. This is the reason for a somewhat extended treatment of the geometry translations, which are executed by the CAD4 programs.

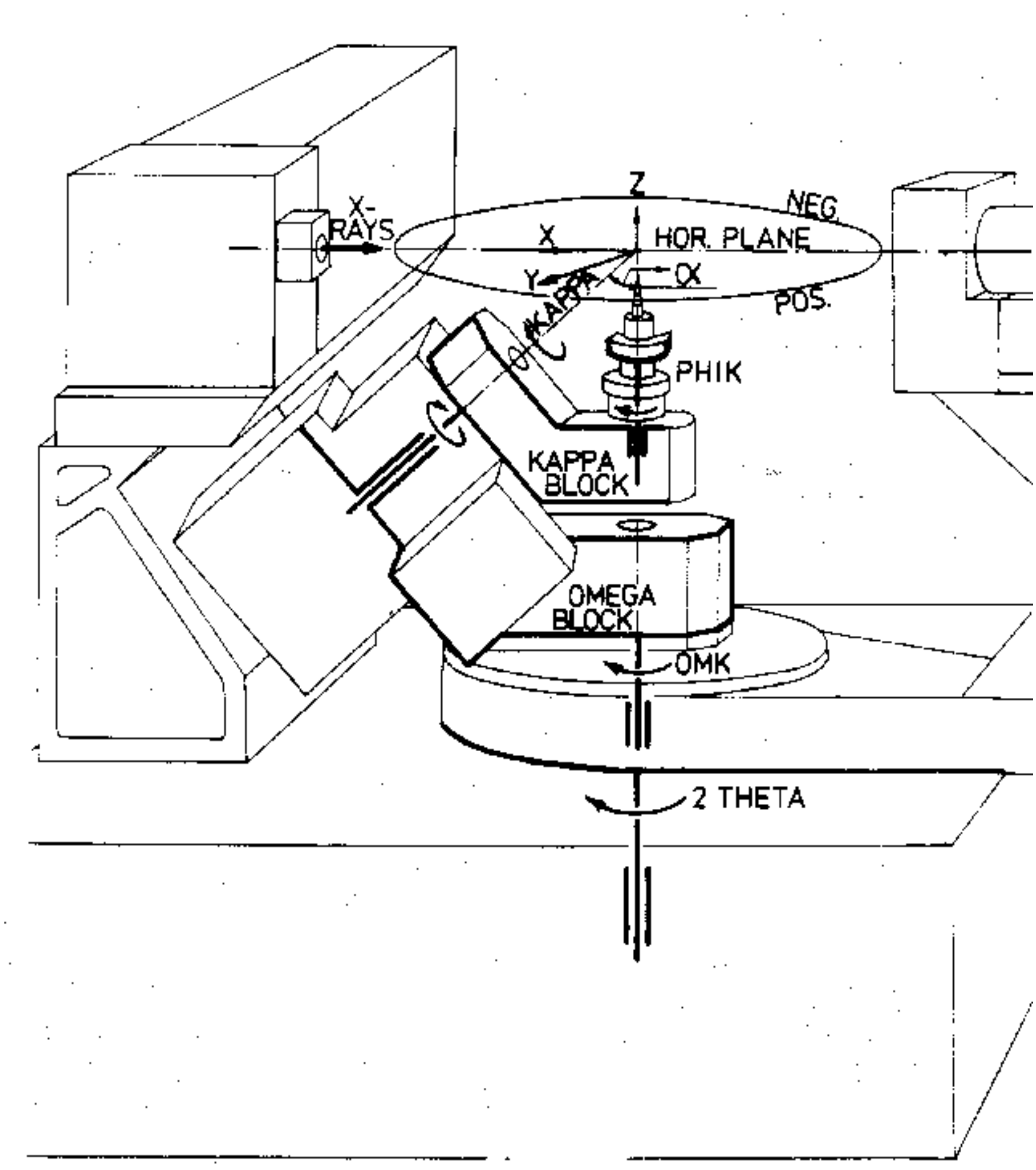
The heart of the CAD4 diffractometer is the kappa goniometer. It carries the goniometerhead, which keeps the crystal in the center of the diffractometer. The kappa goniometer consists of a combination of three parts, bearing the three rotation axes. All axes intersect in the center of the diffractometer. The goniometerhead is mounted on the phi axis, the angle of rotation is called Phik), which is supported by the kappa block. The kappa block can be rotated about the kappa axis (Kappa) being carried by the omega block. In turn, the omega block can be rotated about the omega axis (Omk) being carried by the base plate of the diffractometer. The angle included by the omega axis and the kappa axis, alpha, is = 50°. The angle between the kappa axis and the phi axis is also 50° and the goniometer can therefore access all directions in Chi within ca. 100° of the zero position. This geometry gives enhanced setting flexibility over the traditional Eulerian cradle while simultaneously the obscuration caused by the mount is drastically diminished.

The plane through the center of the diffractometer and perpendicular to the omega axis will henceforth be denoted as the horizontal plane. The position and the intensity of the diffracted X-rays are recorded in this plane. Thus the primary beam is in this plane, pointing towards the center of the goniometer. The vector which is directed from the center of the goniometer towards the X-ray source, is used as the X-axis of the Cartesian coordinate system X, Y, Z. The Z-axis is directed upwards along the omega axis and the Y-axis completes a right-handed set of axes (fig.II.1).

In addition to the goniometer the diffractometer contains a two-theta axis (2Theta) which supports the detector. The two-theta axis coincides with the omega axis. This enables the detector to describe an arc with radius R around the goniometer in the horizontal plane. R is minimally 173 mm and can be extended to 368 mm with a standard tool. For applications needing extremely high spatial resolution of the diffracted beams an optional tool to extend R to 600 mm is available.

The zero position of the axes kappa, omega and two-theta are defined in terms of the geometry of the instrument. The point in kappa rotation, where the phi axis and the omega axis coincide is defined as Kappa=0. The position Omk=0 is defined as the point in omega rotation where Kappa lies in the plane through X and Z and the kappa block is opposite to the direction +X. 2Theta=0 is established as the point in theta rotation where the center (it should be noted that the center of the detector is defined by the slit system in front of it) of the detector lies in the plane through Z and X and the detector is opposite to the direction +X. An arbitrary definition is used for Phik=0, namely the point in the phi rotation where the key on the goniometerhead mount parallels the +X-axis, whereas Kappa=0 and Omk=0.

Starting from Kappa=0 and Omk=0 the definitions of positive rotation directions are given. Positive rotation about theta, omega and phi moves a vector from Y towards X. A positive rotation about kappa moves a vector from Y towards a position below the horizontal plane.



Mechanical alignment

Alignment of the diffractometer can be divided into mechanical and primary beam alignment. Primary beam alignment is treated in the sectipon "Alignment of the diffractometer". Mechanical alignment is the responsibility of the manufacturer and the local service organization, and it includes the following points:

1. Intersection of the goniometer axes in one point. This is checked by doing rotations about the phi, kappa and omega axis using a small sphere, which is mounted on the sample holder. The sphere should stay in its place upon the rotations.

2. Equality of the angles Alpha in the omega and kappa block. Only if this condition is satisfied, the phi and omega axis can be positioned so as to coincide. This is determined by the following procedure: a cylindrical rod is

mounted on the sample holder and aligned accurately in Phik. Kappa is set to zero. The rod may not move out of position, when omega and phi rotations are done.

3. Positioning of the collimator holder and determination of Omk=0. A cylindrical rod can be positioned in the horizontal plane pointing towards the center of the goniometer by adjustment of the collimator holder. This is measured with a distance measuring gauge, which is mounted on the goniometerhead. The goniometerhead is positioned at various angles and the distances to the rod are compared. When this rod is aligned accurately, this set-up can be used to determine Omk=0.

4. Determination of 2Theta=0. In principle, the aligned rod in the collimator holder (3) can also be used to determine 2Theta=0, but it is found to be done more conveniently using X-rays (see "Alignment of the diffractometer").

In the manufacturing stage the equipment is of course subject to many other checks, such as the coincidence of the omega and theta axes, angular accuracy of all rotations and positioning of the center of the detector in the horizontal plane. The CAD4 is designed to maintain the accuracy on these points during normal shipment and usage.

Actual value of the angle Alpha

During factory check-out and alignment of the goniometer the angle Alpha is measured very accurately. The actual value of Alpha has to be entered in the software, since it influences geometry translations. The program GONCON should be used to add the values of the specific constants CON1, CON2 and CON3.

CON1 = $\sin^2$(Alpha)

CON2 = cos (Alpha)

CON3 = $\cos^2$ (Kappa_{max}/2) * $\sin^2$(Alpha)= $\cos^2$ 89. * $\sin^2$(Alpha)

The function $\cos^2$ 89 in CON3 serves to prevent the kappa-block to pass through Kappa = 180º. In special cases it can be changed to limit the Chie range available under CAD4 program control to another value than the standard approx. 100 degrees.

Aperture unit

The aperture unit in front of the detector contains a number of slits, which can be positioned one at a time using CAD4 program control. The slits are held in a rotating disc, which is coupled to an encoder. For every aperture unit the encoder positions are different. These positions are determined individually during the manufacturing. A list of these positions accompanies each aperture unit and the program GONCON should be used to enter these values in the software.

Rotation about an axis in the coordinate system X, Y, Z

The aim of the following sections of this section is to provide a better understanding of the actions taken by the CA04 programs to execute the geometry translation instructions. The description is greatly simplified by introduction of shorthand notations to describe the rotation about an axis. This shorthand notation is defined here.

Positive rotation directions are defined as follows:

the X-axis, turn Z to Y

the Y-axis, turn X to Z

the Z-axis, turn Y to X

The rotation about the X-axis by alpha degrees is denoted as X (Alpha), which represents the rotation matrix for this rotation.

$$\underline{X}(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha) & \sin(\alpha) \\ 0 & -\sin(\alpha) & \cos(\alpha) \end{pmatrix}$$

Similarly the rotation matrices for rotations about the Y- and Z-axes are given by

$$\underline{Y}(\beta) = \begin{pmatrix} \cos(\beta) & 0 & -\sin(\beta) \\ 0 & 1 & 0 \\ \sin(\beta & 0 & \cos(\beta) \end{pmatrix}$$

$$\underline{Z}(\gamma) = \begin{pmatrix} \cos(\gamma) & \sin(\gamma) & 0 \\ -\sin(\gamma) & \cos(\gamma) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Rotation of a sample in the CAD4 geometry

In the zero position of the goniometer a vector $\underline{c}$ is assumed to be attached to the sample. The components of this vector in the X, Y, Z coordinate system are cl, c2 and c3, respectively. Now, the requirement is to derive the mathematical operator, which should be applied to $\underline{c}$, to account for the rotations about the goniometer axes needed to bring this vector in diffracting position.

When the rotations about the phi, kappa and omega axes are Phik, Kappa and Omk degrees, respectively, the total effect of these rotations can be expressed as:

$\underline{c}$(omega, kappa, phi)= $\underline{O}$(Omk) * $\underline{K}$(Kappa) * $\underline{P}$(Phik) * $\underline{c}$

where O (Omk) represents a transformation (rotation) matrix of Omk degrees about the omega axis. The vector $\underline{c}$ contains, as cl, c2 and c3, the components (in Ångstroms) of the reciprocal lattice vector $\underline{h}$ which has components h, k and l in reciprocal space.

The sequence of $\underline{O}$, $\underline{K}$ and $\underline{P}$ reflects the sequence in which the axes are mounted. Phi rotations are done first, with the phi-axis directed along Z. So:

$\underline{P}$ (Phik) corresponds to $\underline{Z}$(Phik). Kappa is directed skewly in the X,Y,Z system, so imagine that the goniometer is rotated about the Y-axis by + (alpha)°. Then the kappa-axis and Z are coincident and a Kappa rotation becomes a Z-axis rotation. Finally, the goniometer is replaced into its original position by another imaginary rotation of -(alpha)° about the Y-axis. Thus $\underline{K}$(Kappa) is equivalent to

$\underline{Y}$(-alpha) * $\underline{Z}$(Kappa) * $\underline{Y}$(+alpha)

The omega-axis is directed along Z and the rotation about it can thus be represented by $\underline{Z}$(Omk).

So the total effect of setting the goniometer to the angles Omk, Kappa and Phik is described by:

$\underline{Z}$(Omk) * $\underline{Y}$(-alpha) * Z(Kappa) * $\underline{Y}$(+a) * $\underline{Z}$(Phik)

Setting a reflection

In the next sections, the process of setting a reflection on the CAD4 diffractometer will be explained. For these calculations it is convenient to go through two intermediate stages, the bisecting geometry and the eulerian geometry.

Setting a reflection in the bisecting geometry

The sample is mounted on the phi-axis, the rotation around this axis will be denoted as Phib. The phi-axis is mounted on a carriage, moving along the chi-arc, which provides the Chib rotation. The phi-axis is perpendicular to the chi-arc and rotates along the theta-axis with respect to the base. The theta-axis is perpendicular to the chi-axis. The zero position of the chi-axis is defined as the point where the phi- and the theta-axes are co-linear. The sample can be rotated by Theta, Chib and Phib.

Setting a reflection in the Eulerian geometry

The sample is mounted on the phi-axis, rotation around this axis will be denoted as Phie. The phi-axis is mounted on a carriage, moving along the chi-arc, which provides the Chie rotation. The phi-axis is perpendicular to the chi-arc and rotates along the omega-axis with respect to the base. The omega-axis is perpendicular to the chi-axis. The zero position of the chi-axis is defined as the point where the phi- and omega-axes are co-linear. Other definitions are equivalent to those used earlier in this section. The sample can be rotated by Ome, Chie and Phie. (Fig. II.2)

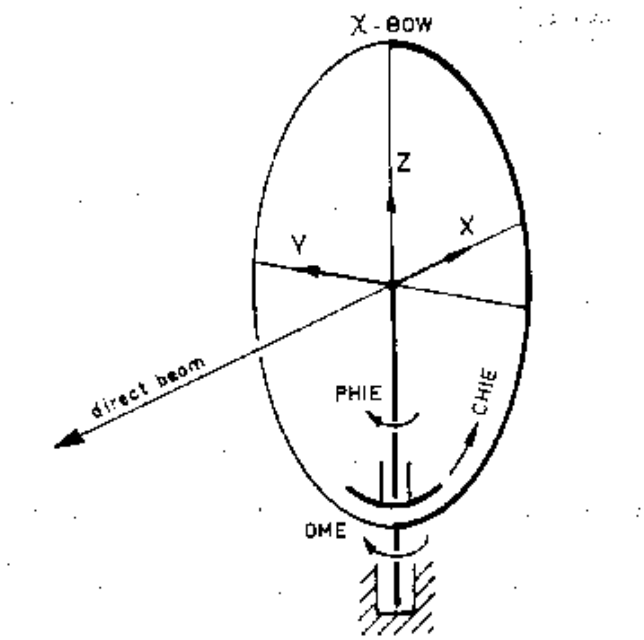


Fig. II-2. Eulerian geometry and relationship with the X,Y,Z coordinate system on the CAD4 diffractometer.

Transformation from Miller indices to kappa geometry

The process of setting a reflection in the diffraction position starts with **the transformation of the Miller indices to the scattering vector.**

An orientation matrix consists of the components of the basic reciprocal grid vectors a, b, and c in the X,Y,Z coordinate system (goniometer angles are zero).

$$R = \begin{pmatrix} a_x* & b_x* & c_x* \\ a_y* & b_y* & c_y* \\ a_z* & \mathrm{b}_z* & c_z* \end{pmatrix} = \begin{pmatrix} R(1,1) & R(1,2) & R(1,3) \\ R(2,1) & R(2,2) & R(2,3) \\ R(3,1) & R(3,2) & R(3,3) \end{pmatrix}$$

An instruction 'HC' is used in the CAD4 program to calculate the components of the scattering vector from given indices. In the terminology of linear algebra this is $\underline{c} = R\ \underline{h}$; or more explictely:

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = R \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

An instruction 'HC' is used in the CAD4 program to calculate the components of the scattering vector from given indices. In the terminology of linear algebra this is c R h; or more explictely:

$$\begin{pmatrix} c_1 \\ \\ c_2 \\ \\ c_3 \end{pmatrix} \begin{matrix} \\ \sim \\ = \\ \\ \\ \end{matrix} \begin{pmatrix} h \\ \\ k \\ \\ l \end{pmatrix}$$

where the ci are components in the diffractometer XYZ coordinate system and h, k and l are components in the reciprocal lattice.

Transformation from the scattering vector to the bisecting position

The next task is to bring the scattering vector c in reflecting position in the horizontal plane. Starting from the zero position of the goniometer, it usually requires a number of rotations.

1. Rotate scattering vector c about the Z-axis until it lies in the Y-Z plane. The rotation angle required is Phib, so the matrix involved is Z(Phib).

2. Then rotate the scattering vector c about the X-axis until a coincidence is obtained with either the +Y-axis if Theta has a positive sign, or the -Y-axis, if Theta has a negative sign. This rotation is denoted as X(Chib).

3. To reach the reflecting position, finally the scattering vector is rotated about the Z-axis. The rotation angle involved is Z(Theta). The series of rotations necessary to set a reflection in Bisecting geometry is thus:

Z(Theta) * X(Chib) * Z(Phib)

The instruction 'CB' is used in the CAD4 program to calculate Theta, Chib and Phib for setting a scattering vector c (cl, c2, c3) in bisecting position. It uses the following expressions

$$\sin(\mathrm{Chib}) = c_3 / (c_1^2 + c_2^2 + c_3^2)^{½}$$

$$\cos(\mathrm{Chib}) = (c_1^2 + c_2^2)^{½} / (c_1^2 + c_2^2 + c_3^2)^{½}$$

$$\sin(\mathrm{Phib}) = - c_1 / (c_1^2 + c_2^2)^{½}$$

cos (Phib) $= c_2 /(c_1^2 + c_2^2)^{½}$

Psi $= 0$

sin (Theta) $= 0.5 * \text{lambda} * (c_1^2 + c_2^2 + c_3^2)^{½}$

$= 0.5 * \text{lambda} *$ absolute c (Bragg's law)

In addition to the settings as explained in the section on Setting a reflection, there are 4 alternative settings:

A. Rotate the scattering vector c about the Z-axis until it lies in the Y-Z plane, while the Y-component is greater than or equal to zero. Then rotate about the X-axis until coincidence with the +Y-axis is obtained. For this setting theta is positive and ABS(Chib) LE 90.0.

B. Rotate the scattering vector c about the Z-axis until it lies in the Y-Z plane, while the Y-component is less than or equal to zero. Then rotate about the X-axis until coincidence with the -Y-axis is obtained. For this setting theta is negative and ABS(Chib) LE 90.0. A rotation about the Z-axis of 180 degrees brings this setting to type A.

C. Rotate the scattering vector c about the Z-axis until it lies in the Y-Z plane, while the Y-component is greater than or equal to zero. Then rotate about the X-axis until coincidence with the -Y-axis is obtained. For this setting theta is negative and ABS(Chib) GT 90.0. A rotation about the X-axis of 180 degrees brings this setting to type A.

D. Rotate the scattering vector c about the Z-axis until it lies in the Y-Z plane, while the Y-component is less than or equal to zero. Then rotate about the X-axis until coincidence with the +Y-axis is obtained. For this setting theta is positive and ABS(Chib) GT 90.0. A rotation about the X-axis of 180 degrees followed by a rotation about the Z-axis of 180 degrees brings this setting to type A.

The rotation about the scattering vector c itself does not change the orientation of the reflecting plane. This rotation is denoted further as the azimuthal rotation Psi. To ensure identical physical azimuthal rotation on both positive and negative side, rotate the scattering vector c until a coincidence is obtained with the +Y-axis as if it was the (normal-) type A setting. Now a reverse rotation of the scattering vector c about the Y-axis is performed over a distance of the azimuthal rotation angle Psi. The rotation angle involved is denoted as Y(-Psi). The scattering vector c is rotated back to the original Y-direction about the X-axis. The rotation angle required is either 0 or 180 degrees for Theta positive and negative respectively.

The series of rotations necessary to set a reflection is thus

$\underline{Z}(\text{Theta}) * \underline{X}(\text{Dt}) * \underline{Y}(\text{-Psi}) * \underline{Z}(\text{Dt+Dc}) * \underline{X}(\text{Dc}) * \underline{X}(\text{Chib}) * \underline{Z}(\text{Phib})$

where

Dt is either 0 or 180 degrees depending on the sign of sin (Theta) and
Dc is either 0 or 180 degrees depending on the sign of cos (Chib)

Transformation from bisecting to eulerian.

From the previous sections it follows that the movement to be made with the scattering vector to set a reflection is described by equation (1).

$$\underline{Z}(\text{Theta}) * \underline{X}(\text{Dt}) * \underline{Y}(\text{-Psi}) * \underline{Z}(\text{Dt+Dc}) * \underline{X}(\text{Dc}) * \underline{X}(\text{Chib}) * \underline{Z}(\text{Phib}) \qquad (1)$$

where
Dt is either 0 or 180 degrees dep. on the sign of sin (Theta) and
Dc is either 0 or 180 degrees dep. on the sign of cos (Chib)

The general description of the movement, which can be made with the CAD4 diffractometer is given by equation (2).

$\underline{Z}$(Omk) * $\underline{Y}$(-alpha) * $\underline{Z}$(Kappa) * $\underline{Y}$(alpha) * $\underline{Z}$(Phik) (2)

Clearly, these two equations should be connected by an equal sign. The aim is to derive the expressions for Omk, Kappa and Phik for the resulting equation. This poses a problem which can be solved by using an intermediate transformation to Eulerian geometry. As explained in the section on Setting a reflection the movement which can be made in Eulerian geometry is described by (3).

$\underline{Z}$(Ome) * $\underline{X}$(Chie) * $\underline{Z}$(Phie) (3)

In the CAD4 program the instruction 'BE' is used to produce Ome, Chie and Phie from the equality of equations (1) and (3).

The total transformation from bisecting to eulerian geometry is:

Z(Ome)*X(Chie)*@(Phie)=Z(Theta)*X(Dt)*Y(-Psi)*Z(Dt+Dc)*X(Dc)*X(Chib)*Z(Phib)

where
Dt is either 0 or 180 degrees depending on sign of sin(Theta) and
Dc is either 0 or 180 degrees depending on sign of cos(Chib)

Substituting:

Eps = Ome - Theta and
dPhi = Phie - Phib

gives:

Z(Eps)*X(Chie)*Z(dPhi) = X(Dt)*Y(-Psi)*Z(Dt+Dc)*X(Dc)*X(Chib)

Nine equations can be developed:

```
 cos(Eps)*cos(dPhi)-sin(Eps)*cos(Chie)*sin(dPhi) =  St*Sc*cos(Psi)           (1)
 cos(Eps)*sin(dPhi)+sin(Eps)*cos(Chie)*cos(dPhi) =    -Sc*sin(Psi)*sin(Chib) (2)
 sin(Eps)                 *sin(Chie)           =     Sc*sin(Psi)*cos(Chib) (3)
-sin(Eps)*cos(dPhi)-cos(Eps)*cos(Chie)*sin(dPhi) = 0                         (4)
-sin(Eps)*sin(dPhi)+cos(Eps)*cos(Chie)*cos(dPhi) =                 cos(Chib) (5)
 cos(Eps)                 *sin(Chie)           =                 sin(Chib) (6)
                           sin(Chie)*sin(dPhi) =    -Sc*sin(Psi)           (7)
                          -sin(Chie)*cos(dPhi) = -St*Sc*cos(Psi)*sin(Chib) (8)
                           cos(Chie)           =  St*Sc*cos(Psi)*cos(Chib) (9)
```

where
St is either +1 or -1 depending on the sign of sin(Theta) and
Sc is either +1 or -1 depending on the sign of cos(Chib)

From these nine equations the following expressions can be derived:

I sin(Chie) = $k*((\cos(Psi)*\sin(Chib))^2 + \sin^2(psi))^{1/2}$

II cos(Chie) = St*Sc*cos(Psi)*cos(Chib)

III sin(Eps) = Sc*sin(Psi)*cos(Chib)/sin(Chie)

IV `cos(Eps) = sin(Chib)/sin(Chie)`

V `sin(dPhi) = -Sc*sin(Psi)/sin(Chie)`

VI `cos(dPhi) = St*Sc*sin(Chib)*cos(Psi)/sin(Chie)`

where k can be either +1 or -1. In practice k is choosen to have the same sign as Sc*sin(Chib)

The solution above degenerates if both sin(Psi) and sin(Chib) are zero, sin(Chie) will be zero then. Now Eps can be choosen and dPhi calculated from:

VII `sin(dPhi) = -sin(Eps)*cos(Chib)`

VIII `cos(dPhi) = St*Sc*cos(Eps)*cos(Psi)`

Eps will be choosen to be Dc (0 or 180) in practice.

The practical solution to calculate the Eulerian angles is:

equation (9) immediately provides cos(Chie); sin(Chie) is derived from cos(Chie).

cos(Chie)	= St*Sc*cos(Psi)*cos(Chib)	(9)
sin(Chie)	$= k*(\sin^2(psi) + \cos^2(Psi)*\sin^2(Chib))^{1/2})$	(15)

in which k equals +1 or -1. In practice, as described above k is chosen to have the same sign as Sc.sin(Chib)

Once sin(Chie) is determined, (7) and (8) determine dPhi:

sin(dPhi)	= -Sc*sin(Psi) /sin(Chie)	(7)
cos(dPhi)	= St*Sc*cos(Psi)*sin(Chib)/sin(Chie)	(8)
Phie	= Phib + dPhi	(16)

Similarly, equations (3) and (6) produce Eps:

sin(Eps)	= -Sc*sin(Psi)*cos(Chib)/sin(Chie)	(3)
cos(Eps)	= sin(Chib)/sin(Chie)	(6)
Ome	= Theta + Eps	(17)

In addition to the solution Ome, Chie and Phie there exists an alternative solution Ome+180, -Chie and Phie+180. This solution is related to the alternative value of k.

The solution given above degenerates if both Psi=0 and Chib=0. Then Chie=0 and Eps=-dPhi. The Phie and Ome axes are co-linear.

The same holds for Psi=180 and Chib=0. However, now Chie=180 and Eps=dPhi+180.
At this point, it is worthwhile to investigate the influence of the azimuthal rotation.

The amount of Phie and Ome rotation caused by Psi are named dPhi and Eps respectively. When making a Psi rotation, the sample is rotated about the scattering vector c. The angle between c and the phi-axis is 90-Chib. So during the Psi rotation, the phi-axis moves along a cone with a half-topangle 90-Chib, whereas the cone axis lies in the horizontal plane The next table shows the results for 90 degrees steps of Psi (see also Fig. II.3).

Psi=0	Chie=90-(90-Chib)	Eps=0	dPhi=0
Psi=90	Chie=90	Eps=90-Chib	dPhi=90
Psi=180	Chie=90+(90-Chib)	Eps=0	dPhi=-or+180
Psi=90	Chie=90	Eps=-(90-Chib)	dPhi=90

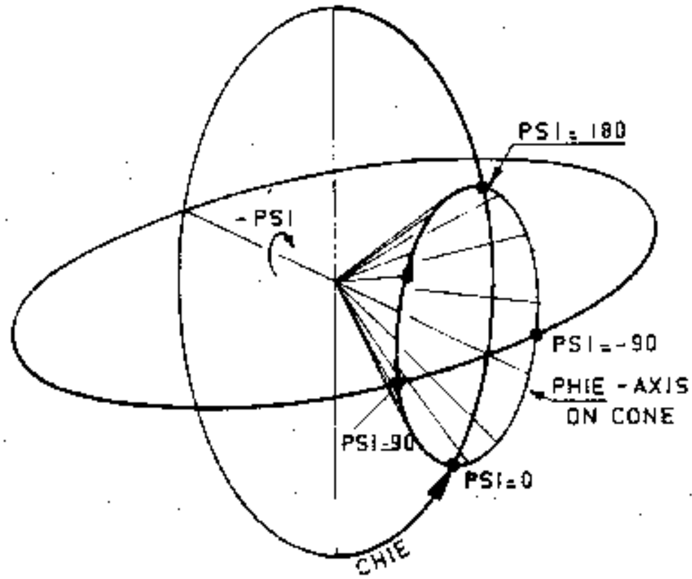


Fig. II.3. Relationship between Psi-angle and Chie-, Phie-setting angles.

Chie moves from under 90 degrees to above 90 degrees and is equal to 90 degrees if Psi = + or -90 degrees, dPhi rotates against Psi over the full 360 degrees. From the table it looks like dPhi = -Psi, but this is only true at the four points selected.

For primary beam alignment it is interesting to note the relations between two settings 180 degrees apart in Psi:

If at Psi = Psi1, the parameters are Chie1, Eps1 and dPhi1, then at
Psi = Psi1 + 180, the parameters are:

Chie = 180 - Chie1, Eps = -Eps1 and dPhi = dPhi1 + 180.

This leads to the statement:

If a reflection is rotated in azimuth by 180 degrees, independent of the starting point, then the phi-axis is also rotated by 180 degrees. The average of the two Chie angles is 90 degrees and the average of the Eps angles is 0 degrees.

One special case is Chib = 90 degrees. In this case the scattering vector $\underline{c}$ coincides with the phi-axis and the solutions degenerate to:

Chie = 90
dPhi = -Psi
Eps = 0

This case is further referred to as the 'top-reflection' case.

Another special case is Chib = 0

Now the solution degenerates to:

Chie = k * Psi
dPhi = -k * 90

Eps = k * 90
k = +1 or -1.

A reflection, for which Chib = 0, is an 'equatorial reflection'

Transformation from eulerian to kappa geometry

As outlined in the foregoing sections rotation in Eulerian geometry is described by:

$\underline{Z}$(Ome) * $\underline{X}$(Chie) * $\underline{Z}$(Phie)

In Kappa geometry the rotations are represented by:

$\underline{Z}$(Omk) * $\underline{Y}$(-alpha) * $\underline{Z}$(Kappa) * $\underline{Y}$(+alpha) * $\underline{Z}$(Phik)

To obtain the setting angles Omk, Kappa and Phik, the expressions given above are set equal and the resulting equation is solved. In the CAD4 programs this process is initiated by the instruction 'EK'.

$\underline{Z}$(Omk) * $\underline{Y}$(-alpha) * $\underline{Z}$(Kappa) * $\underline{Y}$(+alpha) * $\underline{Z}$(Phik) = $\underline{Z}$(Ome) * $\underline{X}$(Chie) * $\underline{Z}$(Phie)

This can be simplified to:

$\underline{Y}$(-alpha) *$\underline{Z}$(Kappa) * $\underline{Y}$(+alpha) = $\underline{Z}$(Ome-Omk) * $\underline{X}$(Chie) * $\underline{Z}$(Phie-Phik)

Substituting dO for Ome-Omk and dP for Phie-Phik, this equation can be written as:

$$\begin{pmatrix} \cos(\alpha) & 0 & \sin(\alpha) \\ 0 & 1 & 0 \\ -\sin(\alpha) & 0 & \cos(\alpha) \end{pmatrix} * \begin{pmatrix} \cos(\kappa) & \sin(\kappa) & 0 \\ -\sin(\kappa) & \cos(\kappa) & 0 \\ 0 & 0 & 1 \end{pmatrix} * \begin{pmatrix} \cos(\alpha) & 0 & -\sin(\alpha) \\ 0 & 1 & 0 \\ \sin(\alpha) & 0 & \cos(\alpha) \end{pmatrix} =$$

$$\begin{pmatrix} \cos(dO) & \sin(dO) & 0 \\ -\sin(dO) & \cos(dO) & 0 \\ 0 & 0 & 1 \end{pmatrix} * \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(Chie) & \sin(Chie) \\ 0 & -\sin(Chie) & \cos(Chie) \end{pmatrix} * \begin{pmatrix} \cos(dP) & \sin(dP) & 0 \\ -\sin(dP) & \cos(dP) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

After developing the product matrices the following nine equations remain.

$\cos^2$(alpha)*cos(Kappa)+$\sin^2$(alpha)	=	cos(dO)*cos(dP)-sin(dO)*sin(dP)*cos(Chie)	(1)
cos(alpha)*sin(Kappa)	=	cos(dO)*sin(dP)+sin(dO)*cos(dP)*cos(Chie)	(2)
sin(alpha)*Cos(alpha)*(1-cos(Kappa))	=	sin(dO)*sin(Chie)	(3)
-cos(alpha)*sin(Kappa)	=	-sin(dO)*cos(dP)-cos(dO)*sin(dP)*cos(Chie)	(4)
cos(Kappa)	=	-sin(dO)*sin(dP)+cos(dO)*cos(dP)*cos(Chie)	(5)
sin(alpha)*sin(Kappa)	=	cos(dO)*sin(Chie)	(6)
sin(alpha)*Cos(alpha)*(1-cos(Kappa))	=	sin(dP)*sin(Chie)	(7)
-sin(alpha)*sin(Kappa)	=	-cos(dP)*sin(Chie)	(8)
sin (alpha)*cos(Kappa)+$\cos^2$(alpha)	=	cos(Chie)	(9)

From equations (3), (7), (6) and (8) it follows that dO equals dP. Therefore, Delta is substituted for both dO and dP. Furthermore, introduction of the angles ½Kappa and ½Chie proves to be suited to obtain the desired solution.

$\cos(\mathrm{Chie}) = 2*\cos^2(½\mathrm{Chie}) -1 = 1-2*\sin^2(½\mathrm{Chie})$

$\sin(\mathrm{Chie}) = 2*\sin(½\mathrm{Chie})*\cos(½\mathrm{Chie})$

Thus the nine equations will reduce to two sets of solutions, the normal set:

sin(alpha)*sin(½Kappa)	=	sin(½Chie)	(1N)
cos(alpha)*sin(½Kappa)	=	sin(Delta)*cos(½Chie)	(2N)
cos(½Kappa)	=	cos(Delta)*cos(½Chie)	(3N)

and the alternative set:

sin(alpha)*sin(½Kappa)	=	-sin(1/2Chie)	(1A)
cos(alpha)*sin(½Kappa)	=	-sin(Delta)*cos(½Chie)	(2A)
cos(½Kappa)	=	-cos(Delta)*cos(½Chie)	(3A)

If Kappa_N and Delta_N are the solutions of the normal set, then the solutions of the alternative set are $-\mathrm{Kappa}_N$ and $180-\mathrm{Delta}_N$.

The alternative solution in the Kappa geometry is of the same nature as the alternative solution in the Eulerian geometry.

In the normal set there is a one to one relation between Kappa and Chie. Chie covers the range $-100° \leq \mathrm{Chie} \leq +100°$ as Kappa covers the range $-180° \leq \mathrm{Kappa} \leq +180°$.

Equation (lN) can be written as:

$\sin(½\mathrm{Kappa}) = \sin(½\mathrm{Chie}) / \sin(\mathrm{alpha})$
$\cos(½\mathrm{Kappa}) = (\sin^2(\mathrm{alpha})-\sin^2(½\mathrm{Chie}))^{½}/\sin(\mathrm{alpha})$

This clearly shows the requirement that the absolute value of Chie must lie between -2alpha and 2alpha, since $\cos(½\mathrm{Kappa}) \geq 0$.

Substituting sin(½Kappa) in equations (2N) and (3N) reveals of Delta:

sin(Delta)	= cos(alpha)*sin(½Chie)/((sin(alpha)*cos(½Chie))
	= cotan(alpha)*tan(½Chie)
cos(Delta)	= $(\sin2(\mathrm{alpha})-\sin2(½\mathrm{Chie}))^{½}$/((sin(alpha)*cos(½Chie))
Omk	= Ome-Delta
Phik	= Phie - Delta

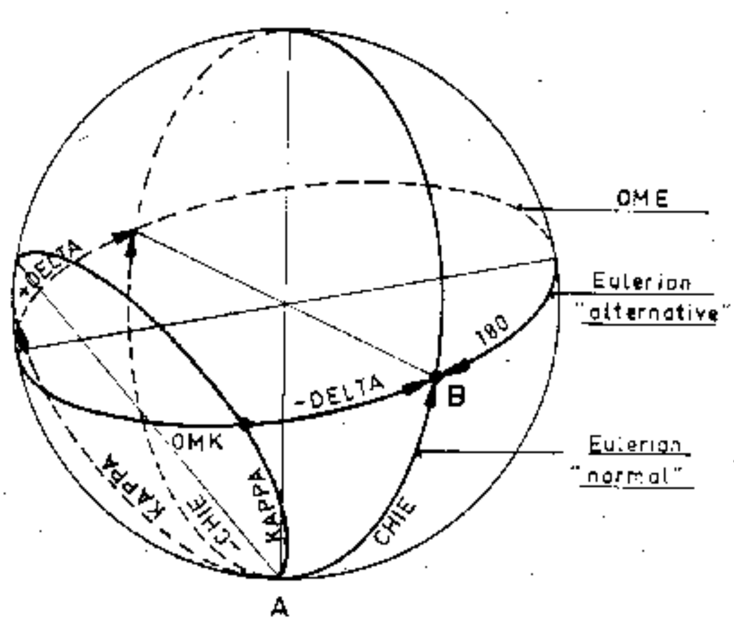


Fig. II.4. Relationship between setting angles for Normal and Alternative Eulerian setting (spherical impression of movement of the sample holder).

In the Eulerian system this only requires Chie movement in the normal solution or -Chie movement and 180 degrees Ome movement in the alternative solution.

In the Kappa geometry, it requires Kappa movement and an Omk movement of -Delta degrees or in the alternative solution -Kappa movement and an Omk movement of -180+Delta degrees.

Finally a list is given of the solutions of Kappa and Delta as function of Chie, provided for alpha = 50.00°

Chie	Kappa	Delta
0.	0.000	0.000
10.	13.066	4.210
20.	26.204	8.509
30.	39.494	12.993
40.	53.036	17.783
50.	66.966	23.034
60.	81.492	28.977
70.	96.965	35.983
80.	114.090	44.756
90.	134.756	57.045
100.	180.000	90.000

Transformation from kappa geometry to Miller indices

The geometry transformations dealt with so far can also be executed in the reversed direction. The instructions used in the CAD4 program are KE, EB, BC and CH.

i. Instruction 'KE' initiates the program to calculate the Eulerian angles from the angles of the Kappa system.

sin(½Chie) = sin(alpha) * sin(½Kappa)

cos(½Chie) = $(\cos^2(\text{alpha}) + \sin^2(\text{alpha}) * \cos^2(½\text{Kappa}))^{½}$

sin(Delta) = cos(alpha) * sin(½Kappa) / cos(½Chie)

cos(Delta) = cos(½Kappa) / cos(½Chie)

Ome = Omk + Delta

Phie = Phik + Delta

ii. Instruction 'EB' initiates the program to calculate the angles in bisecting geometry and Psi form the angles in Eulerian geometry.

Eps = Ome - Theta

sin(Chib) = cos(Eps) * sin(Chie)

cos(Chib) = $k(\sin^2(\text{Chie}) \sin^2(\text{Eps}) + \cos^2(\text{Chie}))^{½}$

sin(Psi) = Sc.sin(Eps) * sin(Chie) / cos(Chib)

cos(Psi) = St.Sc.cos(Chie) / cos(Chib)

sin(dPhi) = -sin(Eps) / cos(Chib)

cos(dPhi) = cos(Eps) cos(Chie) / cos(Chib)

where k can be either +1 or -1. In practice k is choosen to have the same sign as cos(Eps), so Sc becomes SIGN(1.0, cos(Eps))

The solution above degenerates if both sin(Eps) and cos(Chie) are zero, cos(Chib) will be zero then. Now dPhi can be chosen and Psi calculated from:

sin(Psi) = -Sc*sin(Chie)*sin(dPhi)
cos(Psi) = St*Sc*cos(Eps)*cos(dPhi)

dPhi will be chosen to be Phie in practice

iii.Instruction 'BC', serves to initiate the calculation of the x, y and z-components of the scattering vector from Chib, Phib and Theta.

c_1 = -sin(Phib) * cos(Chib) * *2* * sin(Theta)/lambda

c_2 = cos(Phib) * cos(Chib) * *2* * sin(Theta)/lambda

c_3 = sin(Chib) * 2 sin(Theta)/lambda

iv. Instruction 'CHI initiates the program to calculate the Miller-indices from c_1, c_2 and c_3.

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = R^{-1} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

The matrix $\underline{R}^{-1}$ is stored as $\underline{D}$. The rows of the matrix $\underline{D}$ contain the vectors $\underline{a}$, $\underline{b}$, $\underline{c}$ of the direct cell

$$\underline{D} = \begin{pmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{pmatrix}$$

Thus:

$h = a_x * c_1 + a_y * c_2 + a_z * c_3$

$k = b_x * c_1 + b_y * c_2 + b_z * c_3$ or $\underline{h} = \underline{D} . \underline{c}$

$l = c_x * c_2 + c_y * c_2 + c_z * c_3$

Previous: Introduction
Next: Computer systems
