A VERY FAST ORIENTATION DETERMINATION
OF DOUBLY ROTATED QUARTZ CUTS

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ABSTRACT

Determination of orientation of single rotated cuts is very easy because, fortunately, there is only one angle to measure. We can do it so easily because, during a measurement, lattice planes we use, are defined in space as single rotated cuts. Then one angle is needed for knowledge of orientation.

With a doubly rotated cut orientation measurement is much more complicated. To the $\Theta$ angle a second angle called $\phi$ is added. Then we are in a very general situation and the lattice planes we can use are also defined, using the two angles $\Theta$ and $\phi$.

The principle of the goniometer must be changed. Measurements are made using a rotation of the blank during observation.

In such a case, as for the determination of the position of a satellite in space, three measurements are needed. These measurements are made with three different lattice planes. Using a suitable calculation we can find the position in space of the cut. We can see that the quickest way is to choose three lattice planes with the same Bragg angle. That means we do not move the detector during the three observations on the goniometer.

One problem is that if we can measure angles on the goniometer we do not know the actual value of the indexes of the observed lattice planes. Using a trial and error method their exact values are found.

From the values of the scattering factor of the observed lattice planes the sign on the $\Theta$ angle is determined, and from the order of appearance of the observed lattice planes the sign of the $\phi$ angle.

As, with satellite positioning, accuracy of the final determination is increased if more than three lattice planes are used.

INTRODUCTION

We must start saying that the determination of the orientation of a blank cut in a crystal is not a very easy task. Because there is a great difference between the goniometer we use and the crystal we study. The goniometer works in a 2D space and the crystal is in a 3D space. So, from observations made in a 2D space, we have to rebuild a 3D space. A goniometer is always a 2D machine because we measure angles between directions placed on one plane: the graduation goniometer plane. With an X ray goniometer this plane coincides with the plane where we have the incoming and the reflected X ray beam. Fortunately with simply rotated cuts we have two simplifications permitting a very easy measure. It is why we are able to use without any problems our classical goniometers.

The first simplification concerns the blank. According to its definition the blank may be described in a 2D space because the cut is commanded by only one rotation around the $X$ axis.

So the perpendicular to the cut is in the plane defined by the $Y$ and $Z$ axes.

The second one concerns the goniometer. We may choose a lattice plane with a perpendicular also placed on the same $Y$, $Z$ plane. Then the graduation goniometer plane is superposed to plane where the cut is defined (i.e. with an AT cut the (02.2) lattice plane is very useful).

Theoretical Approach

We suppose we are able to determine with a goniometer angles between $N$ the perpendicular to the blank and the perpendicular to some lattice planes $(hkl)_1$, $(hkl)_2$, $(hkl)_3$, .. we call $\rho_1$, $\rho_2$, $\rho_3$, .. these angles.

In the crystal space, positions of these lattice planes are known. They can be expressed with the $\Theta$ and $\phi$ angles of the IEEE convention. According to the number of measured $\rho$ angles a method giving the orientation of the blank may be chosen. With two $\rho$ angles spherical trigonometry is used.
If we have more than two $\phi$ angles we use matrix calculations and then we have in addition the accuracy with which the results are obtained.

**Spherical trigonometry**

Two $\phi$ angles are only measured. Solving some of the spherical triangles presented figure 1, the $\Theta$ and $\Phi$ angles of the blank are obtained. These triangles are constructed with $Z$, the $Z$ direction of the $X$ axis system recommended by the IEEE convention, $N_g$ the perpendicular to the measured blank, $(hkl)_1$ and $(hkl)_2$ the perpendiculars to the used lattice planes.

![Figure 1: Spherical triangles used in the $\Theta$, $\Phi$ determination](image)

The triangle $Z$, $(hkl)_1$, $(hkl)_2$ is directly solved knowing the indexes values of the lattice planes. The triangle $(hkl)_1$, $(hkl)_2$, $N_g$ is solved because the arcs $N_g (hkl)_1$ and $N_g (hkl)_2$ are the measured $\phi$ angles. Then the $Z$, $N_g$, $(hkl)_1$ is solved using results coming from the previous triangles. So, the $\Theta$ and $\Phi$ angles of the blank are calculated. The $\Theta$ angle is the complementary angle of the arc $ZN_g$. The $\Phi$ angle is obtained by addition or subtraction of the angle $N_gZ (hkl)_1$ and the $\Phi$ angle corresponding to $(hkl)_1$ lattice plane.

**Matrix calculation**

Now three $\phi$ angles are measured, introducing a new method matrix calculations. These three $\phi$ angles are associated with three $(hkl)_1$, $(hkl)_2$, $(hkl)_3$ directions. These three directions may be considered as a new axis system. In this new axis system the position of the $N_g$ direction is defined by the three measured $\phi$ angles.

Using matrix calculation (appendix 1) (appendix 2) we pass from this new axis system to the crystal $abc$ axis system. Then the $\Theta$ and $\Phi$ angles of the blank are calculated.

The most important result given by this method is the possibility to determine the accuracy of the measures. Starting from the calculated orientation of the blank, we recalculate the measured angles we have introduced. Differences between observed and calculated values indicate the importance of the error made during either the calculation or the goniometric measurements.

It is also possible to make statistics if more than three lattice planes are observed on the same blank. That gives the possibility to choose planes allowing the best conditions of observation.

**SPECIAL X RAY GONIOMETER**

The methods we present are general and may be applied to any blank orientation of any crystals. The problem is we must be able to observe any lattice plane when we place the blank on a goniometer.

In our laboratory we have developed an adaptation of a four circle goniometer with $\chi = \frac{n}{2}$. The goniometric head is replaced by a supporting plate which holds the blank in position by vacuum suction. This supporting plate revolves around a horizontal axis at high speed (5 rps) and is placed on a mobile arm revolving very slowly around the vertical axis of the goniometer. A stepping motor controls this movement and an absolute coding device gives the exact position of the arm. The X ray detector is fixed onto another arm whose position is known accurately. From the position of the mobile arm and the reading of an X ray meter detector, we determine the blank orientation. This goniometer allows observation of any plane according this single condition:

$$\rho < \Theta \text{ Bragg angle}$$

**MEASURING TECHNIQUE**

The difference between our goniometer and a classical one is that the crystal rotates during the observation. In both cases the reflection is visible only if the observed reticular plane is exactly vertical. This explains why a very fast movement of the supporting plate around the horizontal axis and a very slow movement of the supporting plate arm are combined. When close to a reflection the number of X photons received by the detector varies very quickly, but the envelope of that variation gives a very precise diffraction peak. The half distance between the gravity center of two associate peaks gives the required angle (figure 2).
REFERENCES


APPENDIX 1

Determination of θ and φ of a blank when three lattice planes are used on the goniometer

If three lattice planes (hkl)₁, (hkl)₂, (hkl)₃ are observed on the goniometer, they are associated with the three angles ρ₁, ρ₂, ρ₃. The perpendicular to these observed lattice planes may be called e₁, e₂, e₃. These three directions form a new axis system and they are linked to the crystal reciprocal parameters a*, b*, c* by:

\[
\begin{align*}
\text{e}_1 &= P \cdot \text{a}^* \\
\text{e}_2 &= P \cdot \text{b}^* \\
\text{e}_3 &= P \cdot \text{c}^*
\end{align*}
\]

or

\[
\begin{align*}
\text{a}^* &= P^{-1} \cdot \text{e}_1 \\
\text{b}^* &= P^{-1} \cdot \text{e}_2 \\
\text{c}^* &= P^{-1} \cdot \text{e}_3
\end{align*}
\]

In the \(\hat{e}_1, \hat{e}_2, \hat{e}_3\) axis system the position of \(\hat{N}_g\) is defined by the \(ρ_1, ρ_2, ρ_3\) angles.

Covariant coordinates of \(\hat{N}_g\) in the \(\hat{e}_1, \hat{e}_2, \hat{e}_3\) axis system are:

\[
\begin{align*}
y_1 &= e_1 \cos(ρ_1) \\
y_2 &= e_2 \cos(ρ_2) \\
y_3 &= e_3 \cos(ρ_3)
\end{align*}
\]

And their associated covariant coordinates in the \(\hat{a}^*, \hat{b}^*, \hat{c}^*\) axis system are:

\[
\begin{align*}
x_1 &= P^{-1} \cdot y_1 \\
x_2 &= P^{-1} \cdot y_2 \\
x_3 &= P^{-1} \cdot y_3
\end{align*}
\]

If \(x_1, x_2, x_3\) are covariant coordinates in the \(\hat{a}^*, \hat{b}^*, \hat{c}^*\) axis system, they are contravariant coordinates in the \(\hat{a}, \hat{b}, \hat{c}\) axis system.

From these numbers we obtain the three \(ρ_a, ρ_b, ρ_c\) angles between \(\hat{N}_g\) and the three \(\hat{a}, \hat{b}, \hat{c}\) vectors of the crystal cell.

\[
\begin{align*}
cosρ_a &= x_1/a \\
cosρ_b &= x_2/b \\
cosρ_c &= x_3/c
\end{align*}
\]

The blank orientation is now defined by three angles in the crystal space.

θ angle of the blank is the complementary angle of \(ρ_c\). φ angle is directly calculated from the angle between \(\hat{N}_g\)', the projection on \(\hat{N}_g\) on the XOY plane, and the Y direction.

APPENDIX 2

Determination of the actual values of the (hkl) indexes

The choice of the observed lattice planes is commanded by the position of the X ray detector on the goniometer. But with a given Bragg angle several lattice planes may be observed. Their position in space are different and they differ from each to the others by the position of their indexes. For instance, with a copper X ray radiation the Bragg angle of 51.10° correspond to (40.2), but there are 12 equivalent planes such as : (40.2), (40.2), (04.2), (04.2), ...

During a measurement the value of the (hk.l) indexes of the observed planes is not known. A trial and error method gives their actual values before they are introduced in the matrix calculations.