

# **Sphere of confusion of a goniometer**

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## **Abstract:**

In the diffraction community, the goniometer is a main part of the diffractometer, essential for orienting the samples. To characterize the goniometer, the sphere of confusion (SoC) has been measured. The SoC describes the minimal sphere which enclosed the measurements. This essential data is very important for the diffractometer users. In collaboration with Symetrie Inc., Soleil Synchrotron, and the CEA, the SoC has been measured with three different metrology methods. These three measurement techniques and the associated results are discussed in this article.

## **1-Introduction**

A goniometer has been designed and fabricated in collaboration with Symetrie, Inc. (Nîmes, France) for the Multi-Analysis on Radioactive Samples (MARS) diffractometer at Soleil Synchrotron. This goniometer consists of two rotation (one at 100 rpm) and three translation stages with measured exactitude less than  $\pm 3.0 \mu\text{m}$  according to ISO 230-2 for the sample alignment, mounted on a third rotation stage. This heavy-duty positioning system can carry a 5 kg sample holder and it is enclosed in a 600 mm diameter.

In order to obtain reliable diffraction data, the accuracy of the sample orientation must be done very precisely. The SoC is defined as the minimum spherical volume covering all possible locations of an infinitely small object at all possible goniometer orientations [1]. The SoC is generally described by the diameter of the sphere but sometimes the radius is also used to define the SoC [2]. The accuracy of the goniometer is described by the diameter of the SoC within which the intersection point of the three axes can be contained when

moving any or all of the three axes arbitrarily. In fact, the three axes will in general not intersect at the same point, or not intersect at all, but merely come very close to each other. In this light, when moving all the three axes, the whole measured points, representing a cloud point, define an “error volume” and the SoC value is deduced from this volume. For the acceptance test of the goniometer of Symetrie Inc., different methods of measurements have been realized to determine the point cloud of the “error volume”.

## **2-Description of the measurements methods**

Usually, a ball gauge is used to define the centre of rotation of machine setups with several rotation stages. For the goniometer, the SoC was measured using a ball gauge attached to the Phi-rotation stage. Using the centre of the ball gauge, each point of the cloud is measured and defined thus the shape of the “error volume”. For this operation, the ball gauge should be physically placed in the best possible location on each axes.

There are several methods to measure the centre of the ball gauge. But, the goal consists of always measuring a point (described by 3 co-ordinates) in a Cartesian coordinate system (reference). The choice of the reference is important and should be defined precisely. Results can differ if a reference constructed from the floor or one attached to the system structure has been chosen.

The different methods used to qualify the SoC of the goniometer are: a method by using a coordinate Measuring Machine (CMM), an optical method using an autocollimator and measurements with three linear sensors.

Measurements have been done with the goniometer installed on a CMM machine, then installed on the MARS diffractometer (for the two other measurement methods).

## **3-Results and discussion**

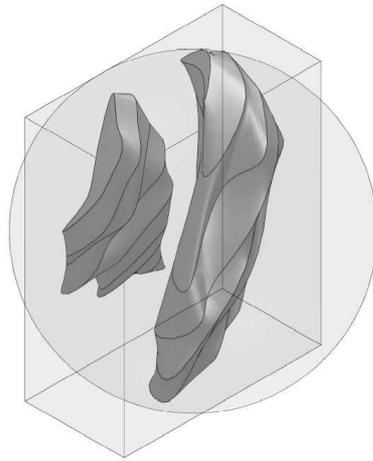
There is more than one method to find the SOC from the point cloud, depending on the method chosen to compute it. For example, one method would be to consider the most remote points of the point cloud and to fit a sphere on these points; another method would be to find the barycenter of the point cloud, and to determine the radius by the distance between the barycenter and the most remote point from it.

Due to the lack of particular shape, the minimal error volume fits badly in a sphere. That is to say if the points measured are fitted in a sphere, a lot of volume is accounted without presence of any points. In our case, the point cloud fits well in a parallelepiped, but this cannot be a general method because in some cases the parallelepiped has a bigger volume than the sphere.

In our case, the method chosen is rather quick and simple, and gives important characteristics in the user reference frame of the minimal volume error: the distance between the most remote points, the range of the projections

of the point cloud on each axis of the reference frame and the middle points of these projections.

To better understand, the point cloud is presented in a 3D plot (figure 1) and the projections of the point cloud are plotted on the planes of the reference frame. This is very helpful to determine some special limited movements range in which positioning error is minimum. Also, these projections allow to distinguish an overall shape of the error point cloud and we can foreseen to compensate a first order component of the error by using the movements of the translation axis of the goniometer.



*Figure 1: plot of the “error volume”.*

The volume enclosed by the parallelepiped containing all the points and having its faces parallel to the user reference is roughly half of the volume of the sphere. A discontinuity appears in the plot that seems to be due to two potential zones that attract the error domain in particular zones of the Khi movement.

The results of the measurements give a distance between the most remote points of 37  $\mu\text{m}$  with the three-sensors method and 39  $\mu\text{m}$  with the optical method.

Knowing better the shape of the “error volume” instead of representing it by the SoC (a sphere and its diameter) allows to take it into consideration when doing an experiment. For example, if the error volume is highly anisotropic, the interesting direction of the sample can be positioned in configuration where the “error volume” is minimal. By this way, this knowledge allows to engineers to develop some instruments, as for example hexapods, complying with the requirements of the scientists.

## **References**

- [1] M.F.Davis, C.Groter and H.F.Kay, On choosing off-line automatic X-ray diffractometers, *Journal of Applied Crystallography* 1 (1968) 209
- [2] He, Bob B. (2009). *Goniometer and Sample Stages*. In *Two-Dimensional X-Ray Diffraction*, pp. 133–150: John Wiley & Sons.

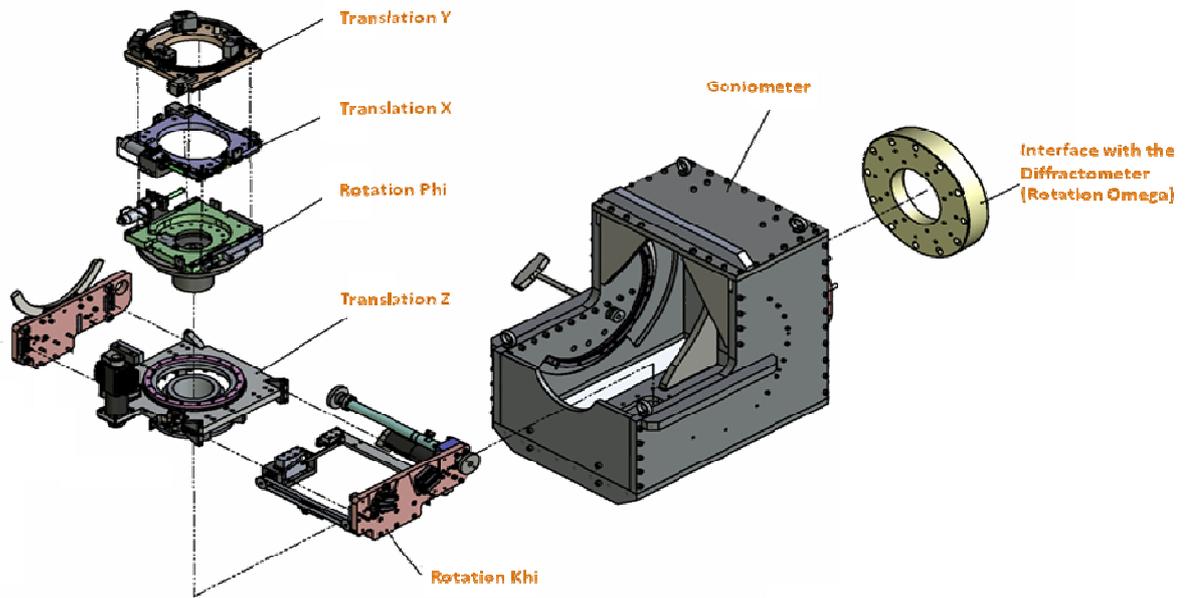


Figure 2: Exploded view of the goniometer

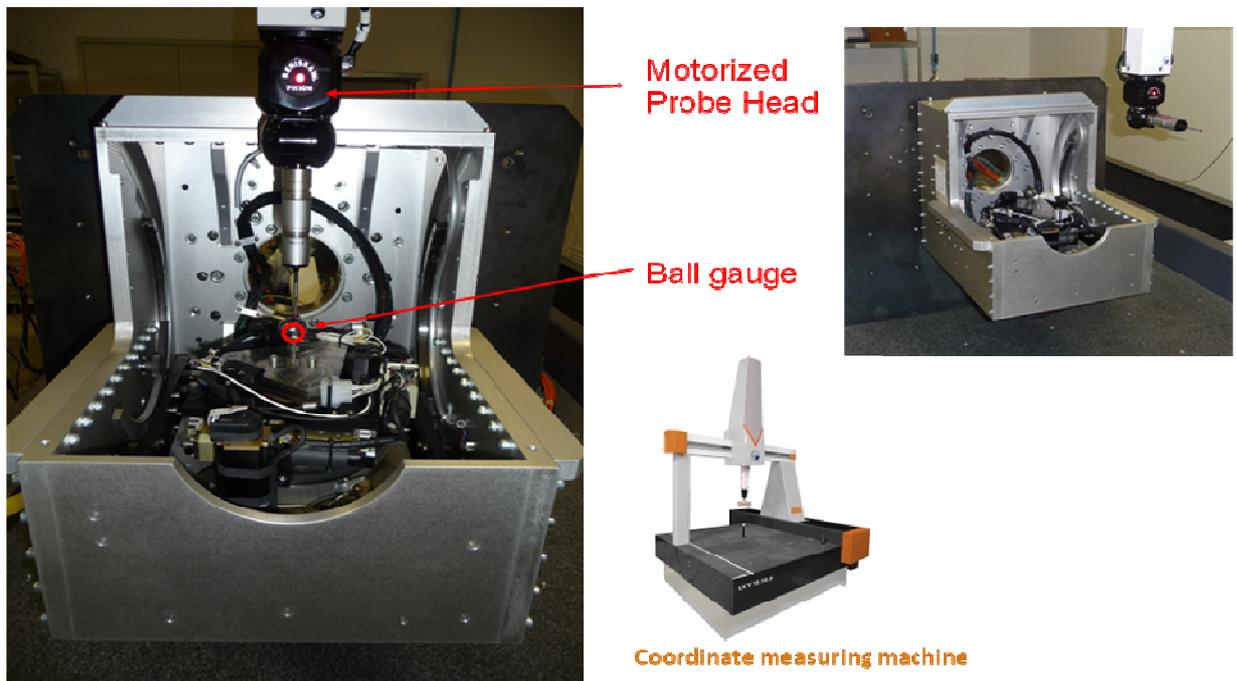


Figure 3: Goniometer on the coordinate measuring machine