A six-circle diffractometry

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Introduction

One of the most popular instruments in x-ray or neutron scattering studies is the four-circle diffractometer. Its angle calculation schemes were developed by Busing and Levy [1]. Despite its popularity, the four-circle diffractometer lacks a sufficient number of degrees of freedom needed for modern x-ray scattering techniques where anisotropic samples, polarization of incoming x-rays, and other geometric factors must be dealt with. For this reason, various types of five-circle and six-circle diffractometers have been developed. Therefore, we have developed a general angle calculation scheme for a diffractometer with four sample-orienting degrees of freedom and two independent detector degrees of freedom (a "4S+2D" six-circle diffractometer shown in Figure 1). This scheme offers several modes of operation [2], each of which can be reduced to most of known diffractometer calculation schemes for various diffractometers including six-circle surface diffractometers and kappa-geometry diffractometers using a set of simple conversion equations. The scheme is numerically tested in a computer program [3]. The central idea is based on the capability (with the extra detector degree of freedom) of constraining a reference vector (which in the surface diffraction case is the surface normal) to a desired orientation with respect to the laboratory frame of reference. The reference vector is not limited to the surface normal but can be any direction of desired or broken symmetry, either structural, electronic, or magnetic in nature.
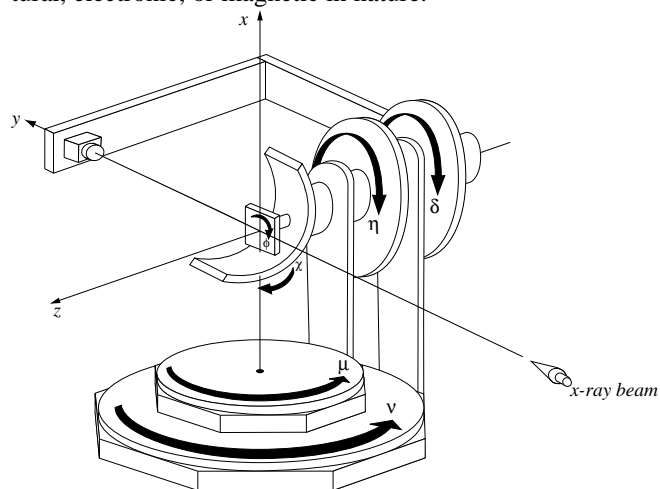

Figure 1: A schematic drawing of the "4S + 2D" diffractometer with all the circles at zero position. The sense of rotations, laboratory frame, and the incoming x-ray directions are shown as arrows.

Definitions of Angles and Pseudo-angles

The notation for the angles (shown in Figure 1) and the coordinate system for the laboratory frame of reference are chosen as consistent as possible with the notations previously used with other diffractometers. When the angles μ and ν are set to zero, the diffractometer is essentially a conventional four-circle where the θ and 2θ angles are named as η and δ, respectively.

The diffractometer circles are not the most convenient angles in controlling the sample orientation since they are defined and built based on mechanical consideration. Therefore, we define a set of pseudo angles, independent of the diffractometer circles, following the scattering geometries. (In the four-circle scheme [1], pseudo angles such as ψ are also used.) The set of pseudo angles and diffracting conditions are shown with an Ewald sphere as shown in Figure 2.
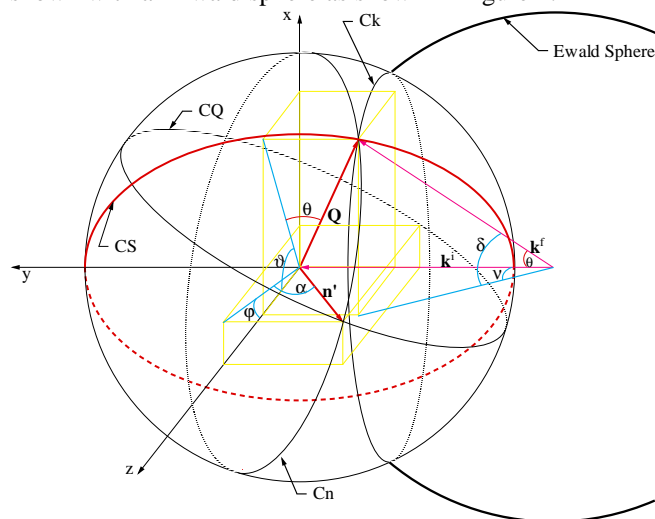

Figure 2: Definitions of pseudo angles shown with the scattering vector and Ewald sphere.

Modes of Operation

The solutions for the various modes of operation are given in detail in [2], and only usage of the modes will be discussed here. In Table 1, the various pseudo and real angles are shown. Since three out of six degrees of freedom must be predetermined in order to obtain a unique solution, one each angle in three columns must be given in advance. Although numerous possibilities exist, in general only a few modes will be needed in a given experimental condition, and the usage will be greatly simplified in real experimental conditions. Most of the solutions for various combinations are given in [2] and those not given can be obtained using the presented equations as needed.

Table 1. Columns of angles used in the calculation scheme. The angles naz and qaz are azimuthal angles for the vectors **n** and **Q**, respectively.

	Det	Ref	Sample	Sample	Sample
1	δ	$\alpha=\beta$	μ	μ	μ
2	ν	α	η	η	η
3	naz	β	χ	χ	χ
4	qaz	ψ	ϕ	ϕ	ϕ

Acknowledgments

References

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[3] SPEC Certified Scientific Software, P.O Box 390640, Cambridge, MA 02139 USA (http://certif.com/) (1998).