Nanometer-level axis of rotation metrology for a high-precision macromolecular X-ray diffractometer

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Abstract. The availability of micro-focused beams at 3\textsuperscript{rd} generation synchrotrons makes collecting X-ray data from macromolecular crystals down to a fraction of micron size possible. This requires using goniometers with nanometer-level errors. Crystal positioning is typically realized with a multi-axis goniometer designed to minimize error motion during rotation of the crystal by the data-collection axis. In this paper, five degree-of-freedom error motions of an air bearing diffractometer data-collection axis are evaluated using a multiprobe method. As spindle errors and artifact out-of-roundness approach equal magnitudes, techniques must be used to distinguish and separate each error. A purpose-built fixture orients a single capacitive sensor in three asymmetrical positions to separate artifact form error from spindle error motion. Metrology results of this air bearing Omega spindle demonstrate synchronous errors of 16 nm radial, 4 nm axial and 0.28 \textmu rad tilt.

1. Introduction

The availability of micro-focused beams at 3\textsuperscript{rd} generation synchrotrons makes collecting X-ray data from macromolecular crystals down to a fraction of micron size possible. This requires using goniometers with nanometer-level errors. Crystal positioning is typically realized with a multi-axis goniometer designed to minimize error motion during rotation of the crystal by the data-collection axis [1-3]. While the expression "sphere of confusion" normally refers to the intersection of several axis (e.g., Omega, Kappa, Phi), it is often misused to describe critical error motions of the data-collection axis. Typically, diffractometers only rotate one axis (Omega) for data collection—the other axes are used to pre-orient the crystal. This means errors of the Omega axis are the most critical as they contribute to unwanted motion of the crystal.

The spindle error motion measurement task is complicated by the nanometer-level magnitude of the errors. As spindle errors and artifact out-of-roundness approach equal magnitudes, techniques must be used to distinguish and separate each error. These errors are sufficiently small that custom-engineered metrology tooling is necessary—error motion testing of the air bearing spindle must reliably characterize errors smaller than 25 nm radial and axial errors. In this paper, five degree-of-freedom error motions of an air bearing spindle data-collection axis of a diffractometer are evaluated using a multiprobe method.
2. Spindle metrology
An expansive amount of research has been published regarding metrology of axes of rotation leading to the development of a definitive resource by Marsh describing the experimental procedures needed to accurately capture error motion of a spindle [4]. The spindle metrology techniques and results described here follow the guidelines outlined by Marsh.

2.1. Background
Schlesinger developed the first systematic approach to testing spindles using contact displacement indicators and a cylindrical test mandrel or testball [5]. Schlesinger pointed out that artifact out-of-roundness and spindle error motions are measured simultaneously so artifact form error must be minimized. As spindle and artifact accuracies approach one another, efforts must be made to distinguish and separate each error.

The reversal technique described by Donaldson provides an elegant mathematical solution for separating spindle error motion from artifact form error [6]. However, in practice, measurement accuracy of this reversal technique suffers from difficulty of implementation. Whitehouse developed a multiprobe technique which avoids some of the complications of reversal [7]. This method, illustrated in Figure 1, requires accurate positioning and alignment of the sensors. Asymmetric angular spacing of the sensors is selected to minimize harmonic suppression and provide results comparable to Donaldson reversal [8].

2.2. Approach
Marsh describes a modification of multiprobe error separation using a single high resolution capacitive sensor positioned at three asymmetrically orientated measurements as shown in Figure 1 [4]. Spindle error motion is characterized by five components—two radial (R_X and R_Y), one axial (Z), and two tilt (α_X and α_Y). Two setups are required to obtain radial and tilt computed from a radial measurement at a low position and another at a high position (100 mm separation). For the low position radial measurement setup, shown in Figure 2, the sensor is moved from 0° to 99.844° and 202.5° to provide radial plus tilt errors at an axial location of 80 mm from the center of the spindle. The chosen orientation angles minimize harmonic distortion of the separation of spindle errors from artifact errors up to a spatial frequency of 225 UPR. In order to resolve tilt components, a second measurement is performed at the high position at an axial location of 180 mm from the center of the spindle as shown in Figure 3. For this measurement, artifact and spindle errors are separated as before using the multiprobe method. The axial measurement, shown in Figure 4, does not require error separation. The artifact's imperfections do not influence the axial measurement except by second-order effects.
2.3. Results
Synchronous low and high radial error separation results are shown in Figure 5 demonstrating 16 nm synchronous error motion (80 mm above spindle center). The growth in error motion when the axial location is increased to 180 mm is a natural consequence of tilt error motion. The tilt error motion, calculated from the two measurements with specified axial separation (100 mm), is shown to be 0.28 µrad in Figure 6. Total synchronous axial component is 2 nm fundamental and 2 nm residual.
3. Horizontal versus vertical orientation

While these measurements were conducted with the spindle axis in the vertical direction, most diffractometers use the Omega axis in the horizontal orientation. This presents a challenge due to fact that positioning systems attached to the rotating member of the Omega axis typically have significant elastic asymmetry.

Prandtl was the first to study the effects of a rotor with elastic asymmetry [9]. The rotor, in the case of most diffractometers, includes all the rotating components attached to the Omega axis (e.g., Kappa and Phi axes) and the XY crystal sample centering table and crystal sample holder. The resulting displacement of an anisotropic elastic rotor under constant gravity load results in second harmonic (2-lobe) error that is often reported for horizontal Omega axes [2,3]. Bryan et al. studied this effect in detail and coined the acronym VISCOORE (Variation in Sag Causes One-for-One Roundness Error) [10]. Cipriani et al. have developed a Kappa diffractometer oriented vertically to almost eliminate the gravity effect and take advantage of the nanometer-level precision of the air bearing Omega axis [11].

4. Conclusions

This paper demonstrates an implementation of five degree-of-freedom precision spindle metrology at the nanometer-level using a multiprobe method to separate artifact error from spindle error. The contribution of typical artifact form error to the total measurement exceeds the spindle error specification. Furthermore, if not properly separated, artifact errors can mask spindle errors—such as 2-lobed artifact errors cancelling 2-lobed spindle errors. A single probe is used with purpose-built fixtures, enabling measurement of axial, radial and tilt spindle error motion components. Metrology results of this air bearing Omega spindle demonstrate synchronous errors of 16 nm radial, 4 nm axial and 0.28 µrad tilt.

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