Precision mechanical design of an ultrahigh-resolution inelastic x-ray scattering spectrometer system with CDFDW optics at the APS

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Abstract. There are many scientific applications, especially involving topics related to the equilibrium atomic-scale dynamics of condensed matter, that require both a narrower and a steeper resolution function and access to a broader dynamic range than are currently available. To meet these important scientific needs, a prototype of a novel ultrahigh-resolution inelastic x-ray scattering spectrometer system has been designed and constructed at undulator-based beamline 30-ID at the Advanced Photon Source, Argonne National Laboratory. This prototype is designed to meet challenging mechanical and optical specifications for performing so-called CDFDW angular-dispersive x-ray crystal optics, which include a central ultra-thin CFW crystal and a pair of dispersing elements. The abbreviation CDFDW stands for: C – collimating crystal, D – dispersing-element crystal (two D-crystals are used in each CDFDW), F – anomalous transmission filter, and W – wavelength-selector crystal [1]. The mechanical design of the ultrahigh-resolution inelastic x-ray scattering spectrometer, as well as the preliminary test results of its precision positioning performance are presented in this paper.

1. Introduction

Many important scientific topics related to the high-frequency dynamics of condensed matter require both a narrower and steeper resolution function and access to a broader dynamic range than are currently available. They are needed for the development of new inelastic x-ray scattering (IXS) spectrometers with improved energy and momentum resolution.

Three effects in the Bragg diffraction of x-rays in backscattering geometry from asymmetrically cut crystals have been observed in [1]. (1) Exact Bragg backscattering does not take place at normal incidence to the reflecting atomic planes. (2) A well-collimated beam is transformed after the Bragg reflection into a strongly divergent beam with a reflection angle dependent on the x-ray wavelength (an effect of angular dispersion). (3) Parasitic Bragg reflections accompanying Bragg backreflection are suppressed. These observations provide a radically new method for monochromatization of x rays not limited by the intrinsic width of the Bragg reflection. However, there are many optomechanical design challenges on the road to turning a CDFDW optical configuration into a practical instrument [1-3].
Based on the above observations, key components of a novel ultrahigh-resolution IXS spectrometer, monochromator, and analyzer have been designed, built, and tested at beamline 30-ID at the Advanced Photon Source (APS), Argonne National Laboratory (ANL). As prototypes, the new devices are designed to meet challenging mechanical and optical specifications for producing ultrahigh-resolution IXS spectroscopy data for various scientific applications [4,5].

The optomechanical design of the prototypes of the ultrahigh-resolution monochromator and analyzer as well as the preliminary test results of their precision positioning performance are briefly presented in this paper. More details are published in an SPIE conference paper [5,6].

2. The CDFDW x-ray crystal optics

As shown in figure 1, the typical so-called CDFDW angular-dispersive x-ray crystal optics includes a central ultra-thin CFW crystal and a pair of dispersing elements. The abbreviation CDFDW stands for: C – collimating crystal, D – dispersing-element crystal (two D-crystals are used in each CDFDW), F – anomalous transmission filter, and W - wavelength-selector crystal.

Figure 1. Schematic diagram of the typical CDFDW x-ray optics for a monochromator with monolithic D-crystals (left) and comb-style D-crystals (right).

The CFW crystal performs collimation of the incident x-ray beam and serves as a wavelength selector. The dispersing elements, which are strain-free mounted monolithic crystals (figure 1, left) or comb-style crystals (figure 1, right) are used to achieve the effect of angular dispersion in exact backscattering from crystal atomic planes. The reflecting crystal planes are almost perpendicular to the working crystal surface in a strongly asymmetric configuration; for instance, with the Si (008) atomic planes for x-ray energy 9.13 keV [4-7]. Figure 2 (left) shows side and rear views of a three-dimensional (3-D) model of the precision mechanical structures for a typical CDFDW x-ray optics for the ultrahigh-resolution x-ray monochromator with comb-style D-crystals.

Figure 2. Left: A 3-D model of the precision mechanical structures for a typical CDFDW x-ray optics. Right: A 3-D model of the base stages for the alignment of the whole CDFDW optics (except the base vertical axis tip-tilting stage).

3. Precision stages design

3.1. Base stages for the CDFDW x-ray monochromator and analyzer

The novel IXS spectrometer prototype consists of two similar sets of CDFDW x-ray optics: one set for the x-ray monochromator, and the other set acting as an x-ray analyzer. To align the whole CDFDW optics to the incoming x-ray beam, the base plate of the CDFDW optics is manipulated by a set of base stages, as shown in figure 3. The base vertical axis tip-tilting stage is not shown in this figure.
The base horizontal rotary stage is a stepping-motor-driven precision goniometer Kohzu™ KTG-15. It is mounted on the carriage of the Kohzu™ high-load-capacity vertical and horizontal stages KHI-4SK. An APS-designed motorized base vertical rotary stage provides an interface between the base stages and the optical table, as shown in figure 4 (right).

3.2, Modular flexure stage groups
Each of the CDFDW optics subassemblies includes 13 positioning stages. A total of 26 precision positioning stages are integrated in the monochromator/analyzer prototype for the IXS spectrometer instrument. Eighteen of them are APS-designed, customized special stages.

Two types of flexure elements are applied for the CDFDW optics precision alignment and positioning: the commercial flexure pivots and Argonne-developed laminar overconstrained weak-link mechanisms. Compared with traditional kinematic flexure mechanisms, laminar overconstrained weak-link mechanisms provide much higher structure stiffness and stability. The strain-limited overconstrained mechanism is a stacking structure with thin-metal weak-link sheets manufactured by photochemical machining processes with lithography techniques. The solid complex laminar weak-link structure provides ultrahigh positioning sensitivity and stability [8-10]. Both rotary and linear laminar weak-link elements are commercially available now [11].

There are three flexure-based positioning stages stacked together for each D-crystal to control its pitch angle coarse and fine motion, linear fine positioning, and roll angle adjustment as shown in figure 2. Four sets of such stage modules have been built for the APS monochromator and analyzer prototypes for the novel IXS spectrometer. To achieve a better than 0.002-arc sec positioning repeatability in a 1.1-degree angular travel range, a compact PZT-driven rotary stage Z8-73 for the D-crystal’s pitch angle fine and coarse positioning has been designed using an overconstrained rotary weak-link mechanism developed at Argonne [8-10].

The stage groups for D-crystals are mounted on a vertical base plate with a large angular travel range (up to 180 degrees) around a horizontal rotary axis. A high-stiffness precision linear stage Z8-
72, with a 100-nm closed-loop positioning resolution, has been designed with two sets of laminar overconstrained linear weak-link modules perpendicular to each other to provide multidimensional stiffness for the load (up to 2 kg) with various moment directions.

The CFW crystal is made ultra-thin (200-μm) and is mounted on the holder with minimized induced strain to optimize its diffraction effects.

4. Preliminary test results and summary

A proof-of-principle experiment was performed at the undulator-based beamline 30-ID at the APS with prototypes of the CDFDW-optics-based monochromator and analyzer for an IXS spectrometer in April 2011 [4]. Strain-free monolithic D-crystals manufactured at the APS and characterized using x-ray topography were used in this experiment. An energy scan of the CDFDW monochromator around 9.13 keV was performed by a simultaneous change of the angles of the D-crystals. A 0.65-meV combined energy resolution of the monochromator-analyzer pair was demonstrated in the in-line configuration, as well as sharp tails of the spectral distribution function [4]. The tails were very steep, more than 100 times steeper than the tails of a Lorentzian distribution with the same FWHM.

The commissioning of a complete prototype of the IXS spectrometer with sample stages, goniometers, and a novel collimating optic based on Montel mirrors with a graded multilayer coating (as shown in figure 4), as well as the development of ultrahigh-quality D-crystals is in progress at the APS.

The technical details of the CDFDW x-ray optics and further development of the CDFDW-optics-based IXS spectrometer will be published in separate papers.

5. References

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