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Direct Observation of Resonance Fringes in X-ray Cavity: A Diffraction Experiment

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The idea of using multi-plate crystals to confine incident hard X-rays in a closed loop by means of multiple reflection was proposed more than thirty years ago. The simplest two-crystal plate cavity has been mostly investigated theoretically based on the dynamical theory of X-ray diffraction. A variety of experiments in realizing x-ray cavity resonance have also been proposed and attempted. With the advent of synchrotron radiation, high resolution and time resolved experiments for this purpose has recently been conducted and experimental attempts to observe cavity resonance fringes have been pursued.

Her we report the direct observation of resonance fringes inside the energy gap and the total-reflection range of the (12 4 0) back reflection from monolithic two silicon crystal plates of 25—150um thick and a 40—150 um gap using synchrotron radiation of energy resolution Delta E=0.36 meV at 14.4388 keV. This cavity resonance results from the coherent interaction between the X-ray wavefields generated by the two plates with a gap smaller than the X-ray coherence length. This finding may open up new opportunities for high-resolution and phase-contrast X-ray studies, and lead to new developments in X-ray optics.

Keywords: X-ray optics, N beam diffraction, dynamical diffraction

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The Convergent Beam Method for X-Ray and Neutron Microbeam Diffraction Applications

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In 1977 Wyckoff and Agard published a theoretical paper that indicated the possibility to carry out protein crystallography studies with an x-ray beam convergent in one plane. This was intended to show that an x-ray beam incident on a small protein sample from a line focus x-ray source could be used for such measurements. This observation did not attract widespread attention or application. Following development of practical x-ray focusing optics during the early 90's, beginning in 1996, the use of highly convergent static x-ray beams (as differentiated from slightly convergent beams frequently used with the oscillation method) began to be investigated for diffraction applications. Computational and theoretical bases for such applications followed soon after. These studies concentrated on protein diffraction applications. Extension of the convergent beam method (CBM) to neutron diffraction has also been demonstrated with reported beam intensity gains as high as 100 for single crystal and 500 for powder diffraction from small (~100 μm) samples with highly convergent neutron beams. Systematic studies of convergent beam protein x-ray diffraction and neutron diffraction both for structural and strain distribution studies are underway. This paper will summarize experimental and theoretical results and discuss the potential importance of the CBM for laboratory and possible in situ microbeam diffraction applications.

Keywords: convergent-beam diffraction, protein convergent-beam crystallography, neutron convergent-beam crystallography

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State-of-the-art X-ray Optics for In–house Crystallography and Synchrotrons

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This talk gives an overview on the large variety of different X-ray optics based on single- and multi-layer coatings. We present recent developments in (1) one-dimensionally beam conditioning optics for X-ray diffractometry, (2) two-dimensionally focussing optics for single crystal diffraction and small angle X-ray scattering and in (3) total reflection optics guiding the X-rays of free electron lasers (FEL) as well as conventional synchrotron sources.

Selected aspects on the simulation, preparation and characterization of the optics will be discussed. By calculating the optical properties of the coating the best multilayer material can be found. By simulating the complete beam path X-ray optics can be tailored for the requirements of a special application. Sophisticated improvements in deposition technology allow the precise realisation of the specified parameters during the manufacturing of the X-ray optics. An intense characterization by state-of-the-art optical profilometry and X-ray diffraction ensures the quality of the X-ray optics. The profilometry measures the quality of the shape of the optics substrate and X-ray reflectometry measures both accurate film thicknesses and their lateral gradient. Energy scans at a fixed angle of incidence demonstrate the quality of optics for synchrotron applications.

The impact of modern X-ray optics on up-to-date X-ray analysis will be demonstrated on selected applications of single crystal and high resolution diffraction.

Keywords: X-ray optics, multilayer, instrumentation

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Multilayer Optics for Mo Radiation based X-ray Crystallography

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The fabrication of multilayer optics for Mo Kα, the wavelength of choice for small molecule crystallography, is difficult because for this wavelength the maximum angles of incidence at which a multilayer reflects and the Bragg peak widths are small. Consequently, only a small solid angle and a small fraction of the X-ray source can be captured. The resulting intensity gain compared to a graphite monochromator is often disappointing. However, today's deposition techniques allow for the fabrication of high quality multilayers with a small d-spacing that reflect at large angles of incidence. The resulting capturing angles are large enough to produce intense beams.

In this work we designed, fabricated and evaluated a focusing multilayer optic for Mo Kα X-rays. The optic was comprised of two elliptically bent focusing multilayers, which were arranged in the Montel scheme. The paper shows the design and performance of the optic. For an FR591 rotating anode X-ray generator, a comparison of the multilayer optic with a graphite monochromator showed a 5x intensity enhancement. Especially small and weakly diffracting crystals benefit from the large intensity produced by the optic, as illustrated by diffraction analyses. An application case study using a small crystal showed significantly improved resolution, with $\langle I/\sigma \rangle$ values larger than 10 for resolution shells down to 0.77 Å where $\langle I/\sigma \rangle$ was only 1.5 for the graphite monochromator. The R indices improved by a factor 3 when data down to 0.77 Å were used for the evaluation.

Keywords: multilayer X-ray optics, single crystal X-ray crystallography, small molecules