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SUBMITTED TO: 4th International Conference
on Synchrotron Radiation Instrumentation
Manchester, England 7-15 to 7-19-91

Conf-910730--19
BNL-46647

**Monochromator harmonic content measurements and calculations
at energies above 20keV**

BNL--46647

DE92 002069

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Received by 337
OCT 30 1991

Abstract

Measurements of the harmonic content from single and double crystal silicon monochromators have been made in the 20 to 100 keV range at the X17 Superconducting Wiggler Beamline at the NSLS. These measurements are compared with calculations which estimate the monochromatic beam harmonic content and the detection system efficiency with good agreement.

At high photon energies ($> 20\text{keV}$), the scattering of x-rays from an amorphous scatterer is dominated by the inelastic Compton process. At large scattering angles this will completely overwhelm the more forward directed elastic scattering. The Compton x-ray energy shift is large enough to make the distinction between elastic and Compton scattering unambiguous when a spectrum is acquired with a solid state detector. This shift, which is energy dependent, allows the measurement of the relative harmonic intensity in a way that is not affected by pulse pileup in the detector and electronics.

The present measurements were done to assess the level of harmonic contamination from two monochromator systems both used on the X17 beamline: the single crystal type monochromator for the Digital Subtraction Coronary Angiography project;

*Work performed under the auspices of the U.S. Department of Energy, under contract DE-AC02-76CH00016.

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and the double crystal monochromator being developed for the Multiple Energy Computed Tomography (MECT) project and the Materials Science program.

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Introduction

Synchrotron radiation from bending magnet and wiggler sources can provide intense, collimated white x-radiation. While the white nature of the spectrum allows a choice of energy or range of energies of x-rays for an experiment, the broad band spectrum will contain x-rays at multiples of the fundamental energy (harmonics) chosen by the monochromator and, depending on the lattice planes used, some of those harmonics may be passed. The purpose of the present study was to measure and estimate the level of harmonic contamination in the beams prepared by single and double crystal monochromators.

The single crystal monochromator is that used for the NSLS Coronary Angiography Project^{1,2}. This monochromator has two Bragg case Si (1,1,1) crystals which individually prepare x-ray beams above and below the Iodine K edge at 33.17 keV. The harmonic measurements were initiated because it is suspected that harmonic contamination is responsible for some artifacts present in angiograms of human subjects measured at the NSLS. The effect of harmonics in angiography has been mentioned previously, but was assumed to be negligible.⁵ The harmonics at multiples of 33keV will not be absorbed in the human subjects nearly as much as the fundamental which suffers an attenuation of order 1000 on its path through the body. This heavy absorption of the fundamental will result in an enhanced proportion of harmonic content in the transmitted beam. These harmonics affect the response of the dual beam detector used to acquire the images, resulting in artifacts.

We have also measured and estimated the harmonic content from a Golovchenko type double crystal monochromator which may be used for the Multiple Energy Computed Tomography (MECT) project and materials science.³ This monochromator had two Si (2,2,0) Bragg case crystals for the present measurements. The double crystal device will allow the detuning of the crystals relative to one another. Since the

reflection widths of the higher order reflections are somewhat narrower than the fundamental width, the effect of detuning is to reduce the harmonics at a rate which should far exceed the loss of intensity in the fundamental. We have made measurements with this monochromator at 20, 33, 40 and 80keV with varying amounts of detuning. We have also made estimates of the amount of harmonic content based on calculations.

At the "high" x-ray energies used in the measurements the dominant mechanism for scattering at the 90 degree angle is the inelastic Compton effect. The elastic scattering will be much reduced in proportion to the Compton scattering. This may seem to defeat the purpose of the measurement since the elastic peaks in the spectrum are hardly noticeable. However, the Compton peaks are much stronger and can also be used to estimate the spectral content of the incident beam spectrum. The Compton scattering mechanism is simple to estimate using the Klein-Nishina cross section formula. Also, the energy shift of the Compton scattered beam allows the energy of the incident x-ray to be calculated from the scattering angle.

Finally, the most important benefit of using the Compton peaks to measure the harmonic content arises from the fact that the measurement is free from pulse pileup effects. With a synchrotron source, the incidence of pileup is much more noticeable due to the pulsed nature of the source. Within the time resolution of most detectors, the x-rays from each electron bunch will arrive at the same time. Thus if the incident beam could be perfectly monochromatized with no harmonics, pulse pileup in the solid state detector would indicate the presence of harmonics since the piled up pulses would appear at multiples of the fundamental peak height. However, if one uses the Compton peaks, the x-rays scattered have a unique energy which depends on the incident beam energy. In other words, pileup of the Compton scattered fundamental will not appear in the pulse height spectrum at the same energy as the Compton scattered harmonics since the energy shift is not linearly dependent on energy.

Experimental

The experiments were done at the NSLS on the X17B beamline. The single crystal measurements were in the X17B2 Medical Research Facility and the double crystal measurements were done in the X17B1 Materials Science hutch. The source of radiation was the superconducting high field wiggler which was operating at a field strength of 4.4 Tesla. At this field the critical energy of the spectrum is 18.7keV.

In each set of measurements, the monochromatized beam was scattered in a 3mm thick aluminum plate which was placed at a 60 degree incidence angle to the beam. The scattered x-rays were collected by an energy dispersive detector (intrinsic Germanium). The detector was placed in the horizontal plane at 90 degrees to the incident beam. The cross section for scattering (primarily Compton and some elastic scattering) is reduced in the horizontal plane at 90 degrees and limits the count rate to the detector. Total count rate was further controlled by limiting the horizontal incident beam width to give at or below 1×10^4 counts per second. The energy dispersive detector was placed at a distance of 50 cm from the aluminum scatterer. The detector element was 10 mm in diameter and had an active thickness of 7 mm. The scattered spectrum was acquired over a 600 second period and the total count was of the order of 1×10^6 and less.

Calculations

The calculations were based on a set of programs designed to estimate the throughput of perfect crystal optics⁴. These programs calculate the energy and angle throughput for both the sigma and pi polarization components for multiple Silicon and Germanium flat crystals with either Bragg or Laue scattering geometries, dispersive or non-dispersive crystal setting, variable asymmetry, variable thickness, and variable an-

gle offsets. The program has the ability to calculate the transmitted or diffracted beams through each element. The result is a normalized throughput which can be used with another program to estimate the filtered synchrotron flux which will pass through the monochromator for each polarization component. These synchrotron throughputs for the fundamental and harmonics are then used to calculate the amount of scatter from the aluminum plate which can strike the detector. The final step is to estimate the response of the solid state detector to the fundamental energy and the harmonics.

Comparison of Experiment with Calculation

The single crystal monochromator is the simplest to model and from which to measure the scattered spectrum, since there is not the complication of a second crystal which can be detuned. These measurements were done with the raw monochromatized beam and with various sets of aluminum filters and a water phantom filter.

Figure 1 shows a measured scattered spectrum. The solid line shows the spectrum obtained with no absorbers in the incident beam. The dotted line shows the spectrum with a 145mm water absorber. This absorber attenuates the fundamental and enhances the proportion of harmonics in the transmitted beam. The labels above identify where the elastically scattered fundamental and harmonics should appear in the spectrum, and where the Compton scattered (CS) fundamental and harmonics appear. Also present are some escape peaks from the Ge detector and some Pb fluorescence peaks. Note that the elastic peaks are very weak.

The predicted peak values for the Compton scattered fundamental and harmonics are shown with squares for the spectrum with no absorbers and diamonds for the scattered spectrum with the 145mm water absorber. The only adjustable parameter in the fit to the data is a factor which scales the predicted Compton scattered fundamental with no absorber with the measured value. All other predicted values in this plot are

scaled with this same factor. The fit between the measured and calculated scatter peak values is good. The largest discrepancy occurs with the first harmonic (66keV). This harmonic arises from the "forbidden" Silicon (2,2,0) reflection. This reflection is an allowed reciprocal point for the primitive lattice. However, the positions the two atoms occupy in the cell forbid this reflection since the atoms scatter out of phase relative to each other. Bonding charges and thermally induced asymmetric atomic positions contribute to a measurable reflection.

Figure 2 shows a measured scatter spectrum with the double crystal monochromator operating at 40keV. Measurements were also made at 20, 33, 80 and 100keV, but only the 40keV results will be shown here and are representative of the results at the other energies. The solid line shows the spectrum obtained with the monochromator fully tuned in which both crystals are optimized to give maximum throughput. The lower dotted line is the scattered spectrum obtained when the intensity of the fundamental is decreased by 37% from the peak value by adjusting the Bragg angle of the second crystal by a fraction of an arc-second. Again the predicted peak values are shown by squares for the case of no detuning and by diamonds for the 37% detuned case. In this case, the fit of predicted to measured peak values is poor. For the first harmonic, the measured exceeds the predicted value by nearly a factor of 8, while the measured value at the second harmonic is 20 times the expected value!

This discrepancy is further demonstrated by figure 3, which shows the measured and predicted relative harmonic content as a function of detuning of the fundamental. The relative harmonic content is the ratio of the harmonic to the fundamental intensity. The predicted values for the first (80keV) and second (120keV) harmonics are shown by labeled solid lines. The measured data points for the relative content of the first harmonic are shown with squares and for the second harmonic with diamonds. Only when the monochromator is "tuned" is the fit to the data acceptable.

Conclusions

In conclusion, we have measured the harmonic content arising from single and double crystal monochromators at "high" x-ray energies and have been somewhat successful in modeling the expected throughputs for the harmonics in relation to the fundamental intensities. In the case of the double crystal monochromator when the crystals are detuned, the predictions are not so good. It appears that this effect is not dependent on the crystal quality, nor on the relative azimuthal alignment of the crystals. Since measurements were done with filters in the incident beam to drop the power levels, the higher harmonic content is not related to power loading effects. The poorer harmonic rejection may be a fundamental property of the crystals. This behavior is presently being investigated further to discover its origin.

Acknowledgments

This work was performed under US Department of Energy contract number DE-AC02-76CH-00016 to the National Synchrotron Light Source, Brookhaven National Laboratory.

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FIGURES

Figure 1

Scattered spectrum from a Si(1,1,1) monochromator at 33keV fundamental energy with no incident beam absorber and a 145mm water absorber. Data points show calculated values for each harmonic and absorber.

Figure 2

Scattered spectrum from a Si(2,2,0) x Si(2,2,0) double crystal monochromator at 40keV with no detuning and 37% detuning. Data points show calculated values for each harmonic and detuning value.

Figure 3

Calculated and measured effects of detuning the Si(2,2,0) x Si(2,2,0) monochromator on the first and second harmonics. Data points indicate measured values for various amounts of detuning.

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