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Raytracing Simulation of X-Ray Rocking Curve of Diamond Crystal

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Abstract

A ray tracing simulation of the diamond crystal rocking curve was carried out. The simulation results agree well with the measured results. It is also found that, due to the short distance from the source to the diamond crystal, although an asymmetric cut monochromator could expand the beam size and reduce the beam divergence, the resulted beam bandwidth and the final rocking curve width are both fairly large. On the contrast, a silicon 331 asymmetric monochromator gives the best performance because the perfect matching of their diffraction angle. A silicon 333 asymmetric monochromator gives a broad rocking curve width due to the combination of the large beam bandwidth and the large difference of the diffraction angles. To reduce the beam bandwidth, a second monchromator should be used. Although the second monochromator affects the beam size, it may still be large enough to measure the whole diamond crystal for GlueX if the x-ray beam source vertical size is large enough. The crystal curvature contribution to the rocking curve width for each pixel is investigated.

Introduction

The CESS C1 is a bending magnet x-ray station. The distance from the tangent point to the goniometer is 14.5 meters. Due to this short distance, an asymmetric monochromator has to be used to expand the size of the beam and to reduce the beam divergence. The white x-ray beam is not collimated, so the large vertical beam divergence results in a very large beam bandwidth. Furthermore, diffraction angle of the diamond 220 plane is ~19.2 degrees, and the diffraction angle of the silicon 111 plane is ~7.5 degree. The combination of the large bandwidth and the large difference between these two diffraction angles generated a very broad diamond rocking curve peak. To reduce the beam bandwidth, Ken suggested using a second monochromator, and it turned out to be very useful. The measured minimum rocking curve width was reduced from ~250 micro-radians to only ~30 micro-radians after using a silicon 220 monochromator. However, one of the diamond crystal measured at CHESS is believed to have a mosaic spread of 10 micro radians. A 30 micro-radians rocking curve width means that there is still a large contribution from the instrumental broadening. In order to be able to resolve such small rocking curve width, a better performance monochromator should be used in the future mesurements. These monochromators should be either matching the diamond diffraction angle and/or generating smaller x-ray beam bandwidth.

Two silicon monochromator are proposed to be used in the future experiments. They are asymmetric silicon 331 and silicon 333 monochromators. The diffraction angle of silicon (331) plane is very close to that of the diamond (220) plane, which makes it the best monochromator for the diamond 220 rocking curve study. The diffraction angle of silicon (333) plane is also sufficiently close to that of diamond (220) plane and that of the diamond (004) plane. In fact, in our previous experiments at SRS, a silicon 333 symmetric monochromator had been successfully used in the diamond 004 rocking curve studies. But, to our knowledge, no one had used an asymmetric cut silicon 331 or 333 monochromator in the diamond rocking curve studies, so it is necessary to do some theoretical simulation to predict their behaviour in the diamond rocking curve studies. Furthermore, we are not only interested in the diamond 220 rocking curve study, we also want to measure the rocking curves of other diamond diffraction planes. This requires that the x-ray beam bandwidth should be sufficiently small. Approaches that can be used to reduce the beam bandwidth such as using a second monochromator should be also investigated. Therefore, a ray tracing simulation of the diamond rocking curve was carried out. In this report, detailed simulation results are presented.

Theoretical model

The model includes an event generator, a set of monochromators which consists of an asymmetric double crystal monochromator and an optional symmetric double crystal monochromator, a diamond crystal in transmission geometry and a pixel detector which is used to record the topographic images. In figure 1, the layout of the above devices is shown.

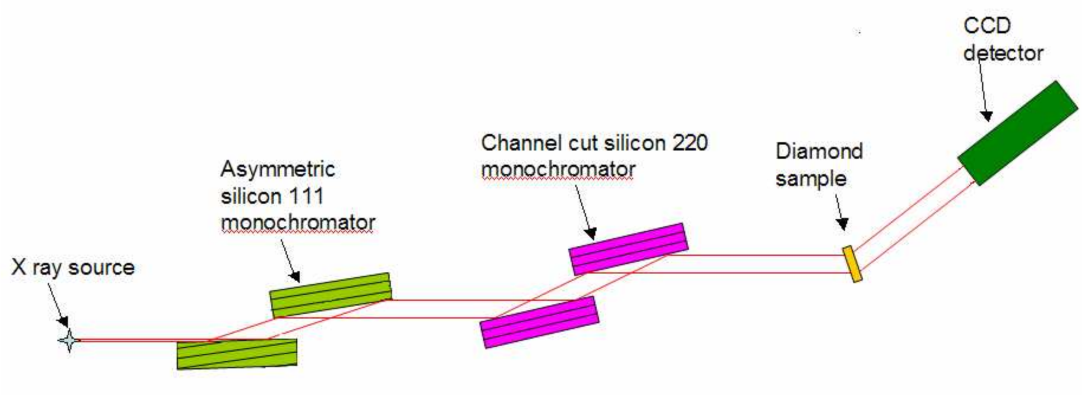

Figure 1. layout of the CHESS C1 rocking curve experimental set up

X-ray photons are generated by the event generator. Each photon has a starting position(x, y, z) and a momentum $\boldsymbol{k}$, both of which are generated randomly. The x-ray source size and the beam divergence are set to comply with the parameters of the CHESS C1 beam line. The vertical source size is 0.7 mm rms and the horizontal source size is 2 mm; the vertical beam divergence is 100 micro radians rms and horizontal beam divergence 1000 micro radians rms; a flat source spectrum over the range of 14.92 - 15.08 keV is used. The first asymmetric cut monochromator is located 10.1 meters downstream of the x-ray source. Although there is no collimator upstream of the monochromator, the monochromator itself act as a collimator due to its limited size. The second optional monochromator is located 1 meter downstream of the first monochromator. The goniometer is located 14.5 meter downstream of the x-ray source. The material, diffraction plane and the asymmetric factor b of the monochromators are selected according to the experimental requirement. The pixel detector is located 0.3 meter down stream of the diamond crystal, which has a pixel size of 20 by 20 microns.

The change in the direction of the x-ray beam diffracted by a perfect crystal is calculated supposing elastic scatting in the diffraction process:

$$\boldsymbol{k_1}=\boldsymbol{k_2}$$

and using the boundary conditions at the crystal surface,

$$k_2\| = k_1\| + G\|$$

where $\boldsymbol{k_1}$ and $\boldsymbol{k_2}$ are the incident and exit wave vectors (outside the crystal), $\boldsymbol{G}$ is the reciprocal lattice vector, and ‖ refers to the component parallel to the crystal surface.

For simplicity, no absorption of the x-ray by the crystal is considered in the simulation. For the monochromators, where only bragg diffraction happens, the criteria for judging if a photon can be diffracted by the monochromator is as follows:

$$\theta - \theta_0 < \Omega/2,$$

where θ is the angle between the incident x-ray and the crystal diffraction plane, θ_0 is the theoretical bragg diffraction angle and Ω is the crystal Darwin width. For the diamond crystal, since the reflectivity profile for transmission geometry follows a gaussian profile, we can not simply judge if a photon can be diffracted or not, instead, the probability of the diffraction is recorded.

Results:

The simulation results are shown by the following figures. In figure 2 and figure 3, rocking curves for perfect diamond (220) plane are shown. In figure 2, the rocking curve width is ~185 micro-radian, while in figure 3, the rocking curve width is ~21 micro-radians. In the former case only a silicon 111 asymmetric cut double crystal monochromator is used, and in the latter case, downstream of the silicon 111 monochromator, a second symmetric silicon 220 monochromator is also used. In figure 4 and figure 5, the bandwidth of the above two cases are shown. It can be seen that if only the asymmetric silicon 111 monochromator are used, the bandwidth can be as high as 13 eV. After introducing the second the monochromater, the bandwidth is reduced to 1.6 eV. The above simulation results agree well with the experimental results of last year, where the minimum rocking curve width are 250 micro radians for one monochromator case and 30 micro radians for two monochromators case[1].

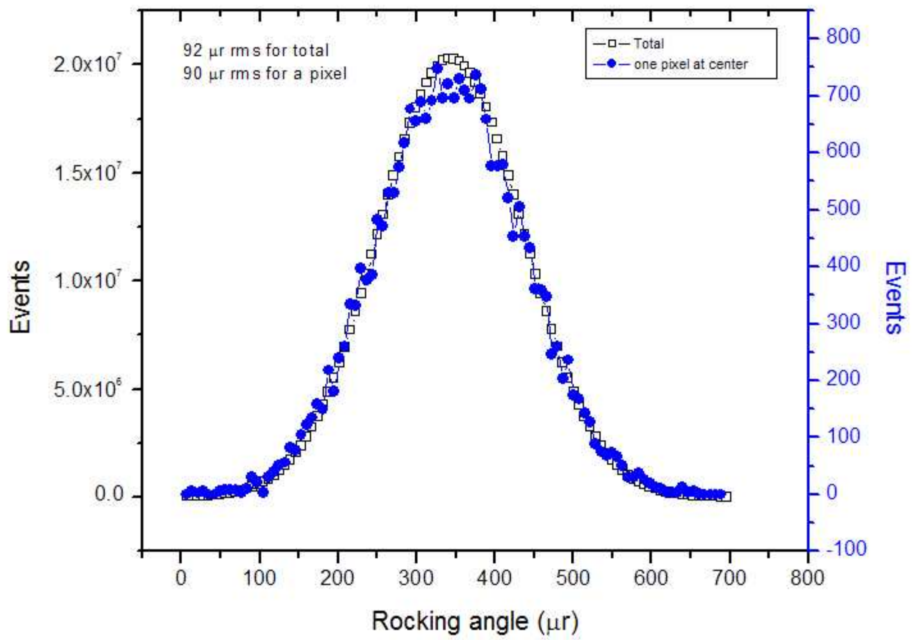

Figure 2. Diamond 220 rocking curves simulated with only an asymmetric cut silicon 111 monchromator. The black square is for the whole diamond crystal, and the blue dot is for a single pixel at the diamond center.

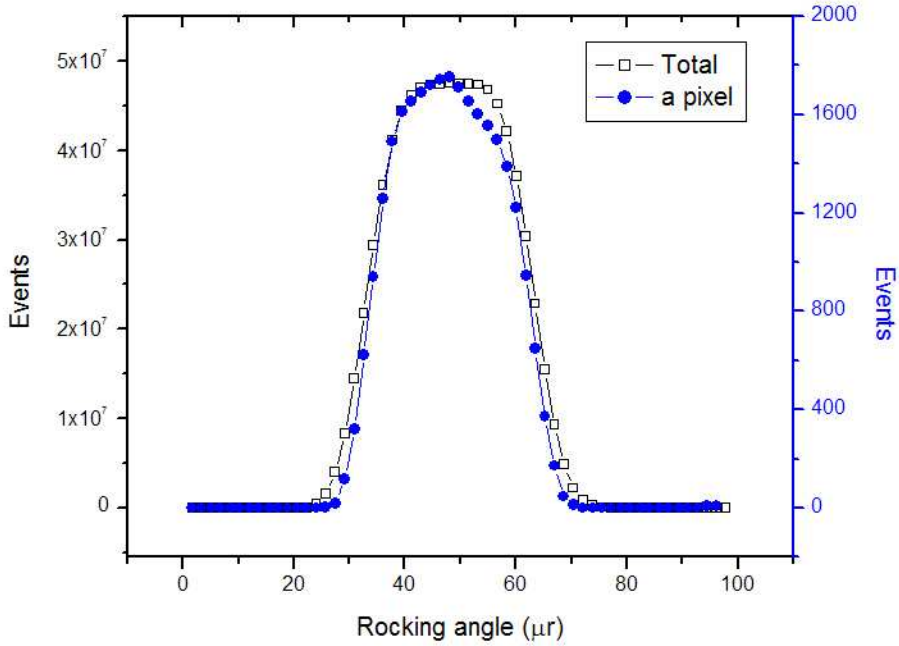

Figure 3. Diamond 220 rocking curves simulated with an asymmetric cut silicon 111 monchromator and the second silicon 220 monochromator. The black square is for the whole diamond crystal, and the blue dot is for a single pixel at the diamond center.

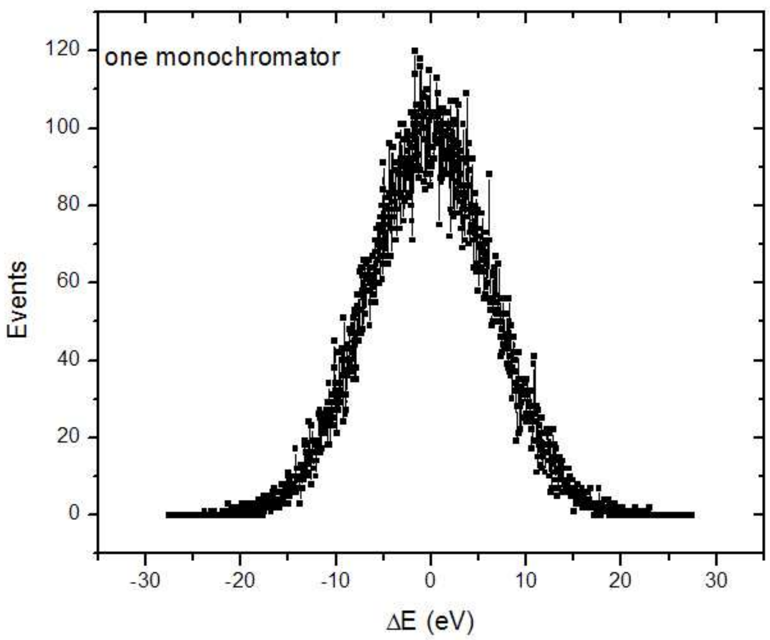

Figure 4. X-ray beam bandwidth when only an asymmetric cut silicon 111 monchromator was used.

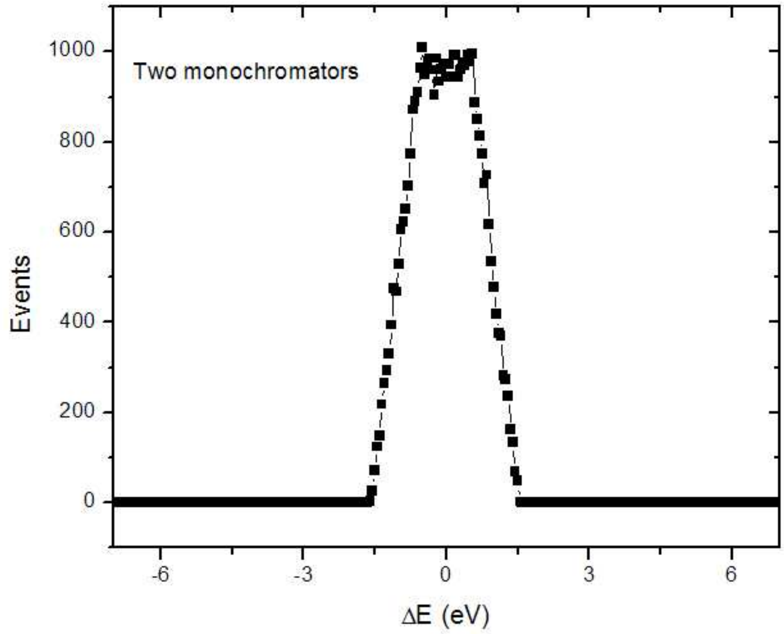

Figure 5. X-ray beam bandwidth when an asymmetric cut silicon 111 monchromator and a silicon 220 monochromator were used.

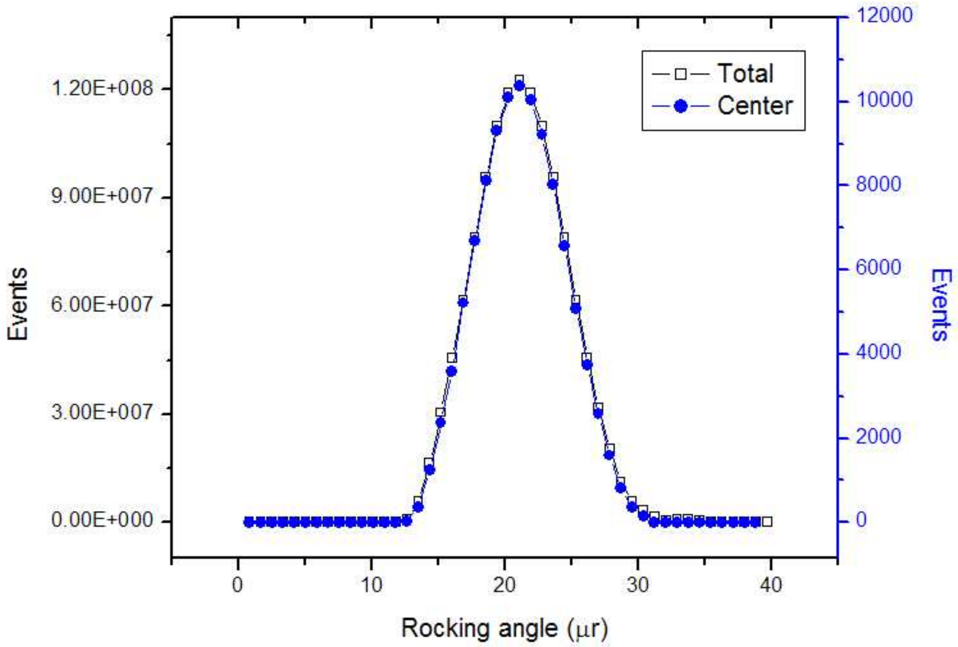

Figure 6. Diamond 220 rocking curves simulated with only an asymmetric cut silicon 331 monchromator. The black square is for the whole diamond crystal, and the blue dot is for a single pixel at the diamond center.

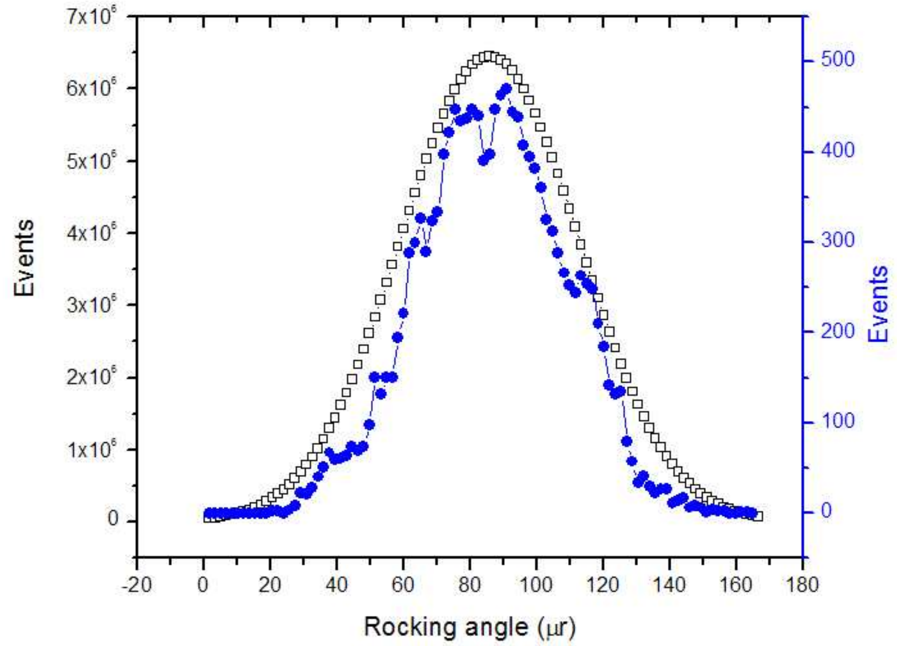

Figure 7. Diamond 004 rocking curves simulated with only an asymmetric cut silicon 331 monchromator. The black square is for the whole diamond crystal, and the blue dot is for a single pixel at the diamond center.

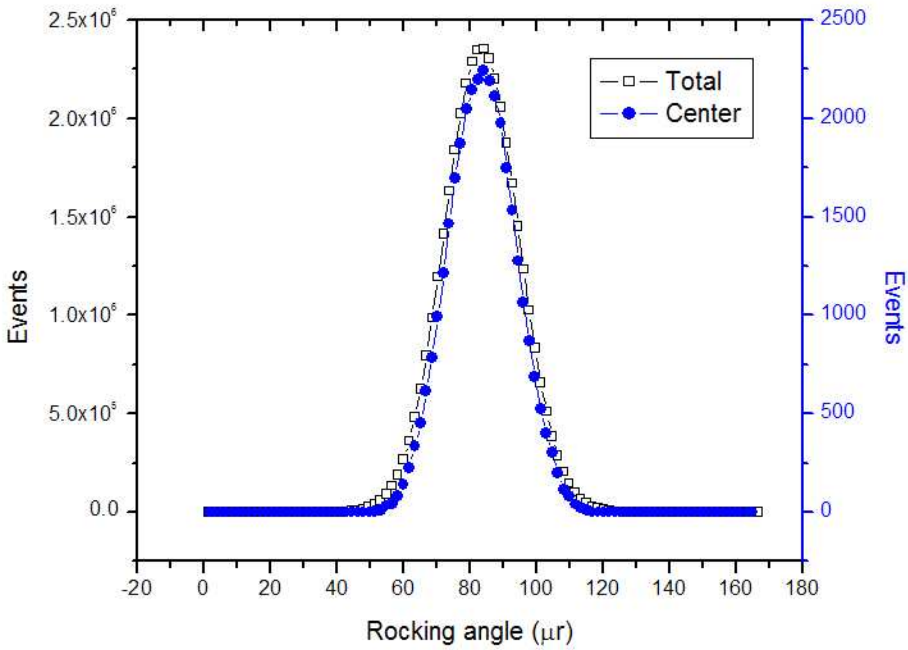

Figure 8. Diamond 220 rocking curves simulated with only an asymmetric cut silicon 333 monchromator. The black square is for the whole diamond crystal, and the blue dot is for a single pixel at the diamond center.

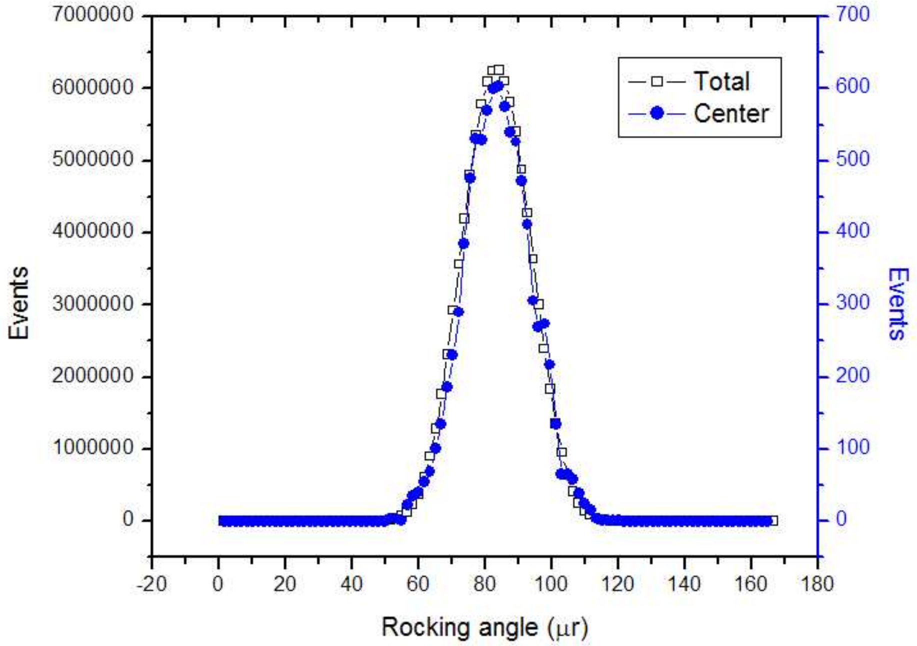

Figure 9. Diamond 004 rocking curves simulated with only an asymmetric cut silicon 333 monchromator. The black square is for the whole diamond crystal, and the blue dot is for a single pixel at the diamond center.

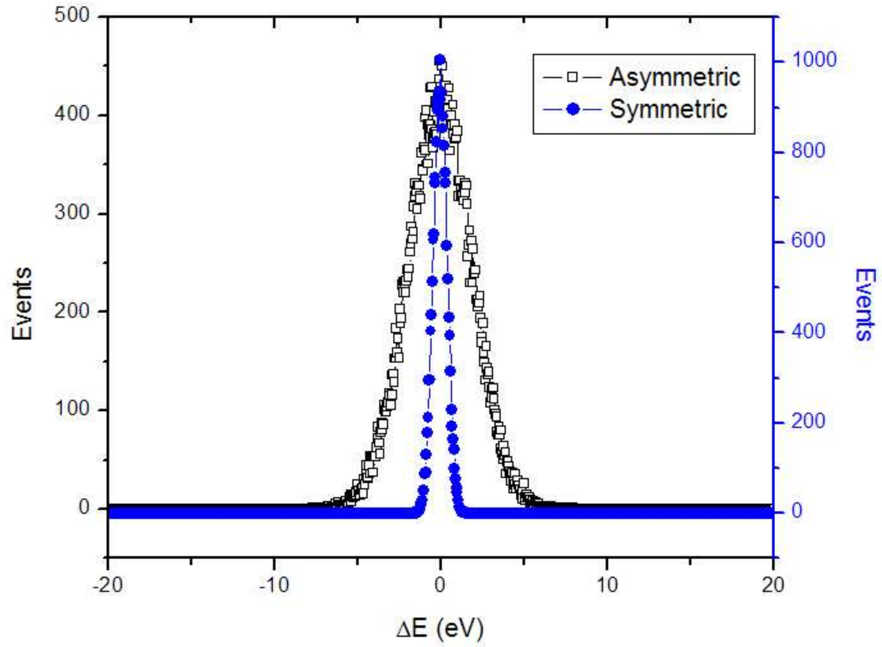

Figure 10. X-ray beam bandwidth a) black square is for an asymmetric cut silicon 333 monchromator, and the distance from the source to the diamond crystal is 10.1 meters. b) blue dot is for a symmetric cut silicon 333 monchromator, and the distance from the source to the diamond crystal is 80 meters.

In figure 6 and figure 7, rocking curves for perfect diamond crystal with an asymmetric cut silicon 331 monochromator is shown. It can be seen that the rocking curve width is quite small, only ~7 micro-radians. So it is well suited to be used to assess the diamond 220 rocking curve. However, when we use this monochromator to assess other diamond diffraction plane, for example the (004) plane, the resulted rocking curve width is rather large (shown in figure 7). This again is caused by the combination of the diffraction angle difference and the large bandwidth of the x-ray beam.

In figure 8 and figure 9, rocking curves for perfect diamond crystal with an asymmetric cut silicon 333 monochromator is shown. It can be seen that the rocking curve width are a little bit large, around 20 micro-radians for both diamond 220 and 004 plane. Therefore, an asymmetric silicon 333 monochromator alone is not suitable for the diamond rocking curve studies.

From the above simulation results, it can be seen that, only silicon 331 monochromator gives a small rocking curve width for the diamond 220 diffraction. Although a silicon symmetric 333 monochromator gives very narrow rocking curves when used in Daresbury, SRS. An asymmetric cut silicon 333 monochromator with a short source crystal distance still gives large rocking curve width. The reason for that is the large bandwidth. In figure 10, the bandwidth for the above two cases are shown, it can be seen that the bandwidth for the latter is much larger.

To reduce the beam bandwidth, we can use another monochromator located downstream of the first monochromator. One thing we noticed from last year's experiments is that the beam size is reduced by the second monochromator, so that the beam is no longer big enough to cover the whole crystal. Two possible reasons are responsible for this. The first one is that the second monochromator size is too small, it self act as a collimator to reduce the beam size. The second one is, because the first monochromator is an energy dispersive device, after passed the first monochromator, the x-ray directions become correlated with their energy, hence the second monochromator cut the beam bandwidth as well as the beam size. However, if the second monochromator is big enough, the beam size will not be a problem for our experiment. This is because the x-ray source size is on the level of 0.7mm rms and the first monochromator expand the beam size by a factor of b. For example, for the silicon 111 monochromator used last year, the factor b is 8.5, so the beam size will be around 6 mm rms. And our crystal have only a 5 mm vertical size, therefore it will not affect our experiments. Indeed, if the x-ray source is a point source, a very small vertical beam size will result in a very small beam size at crystal position if we used the second monochromator. The horizontal beam size is not affected by the monochromators. In figure 11, the vertical beam sizes at the diamond crystal position are shown, it can be seen that the simulation results agree well with the above statements.

By using the combination of a silicon 331 asymmetric monochromar and a silicon 333 symmetric monochromator, the diamond 004 rocking curve width is reduce dramatically from 56 micro radians to only ~7 micro radians, as shown in figure 12. However, at the same time, the beam intensity is reduced dramatically.

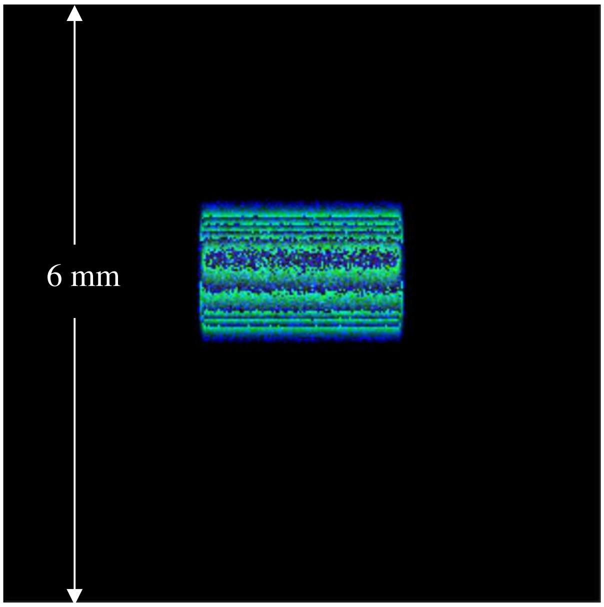

Figure 11. Simulated topograph. (the source vertical size is set to zero.)

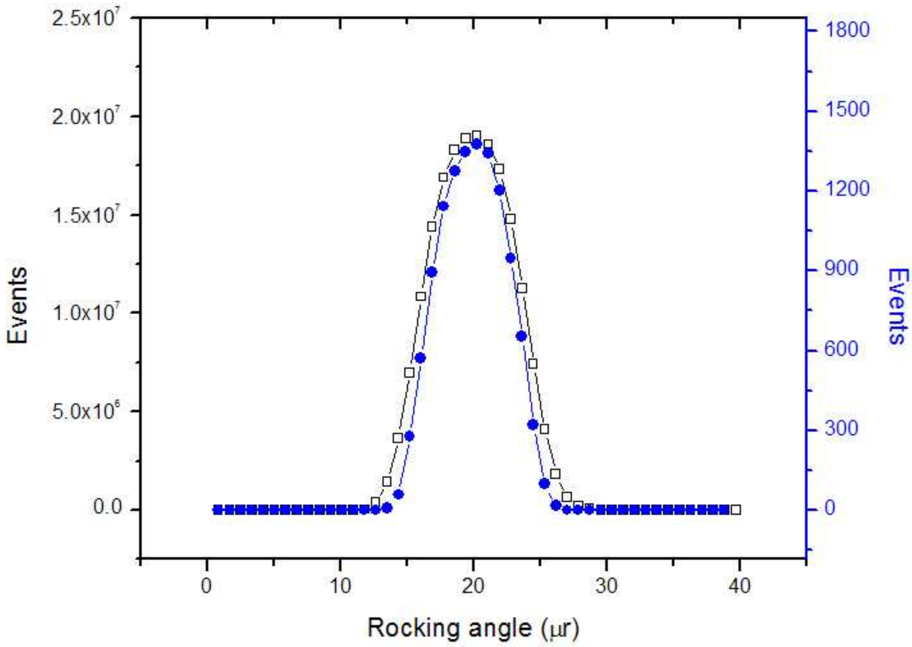

Figure 12. Diamond rocking curves. (with an asymmetric cut silicon 331 monchromator and a second symmetric cut silicon 333 monochromator. The back square is for the whole crystal and blue dot is for crystal center.)

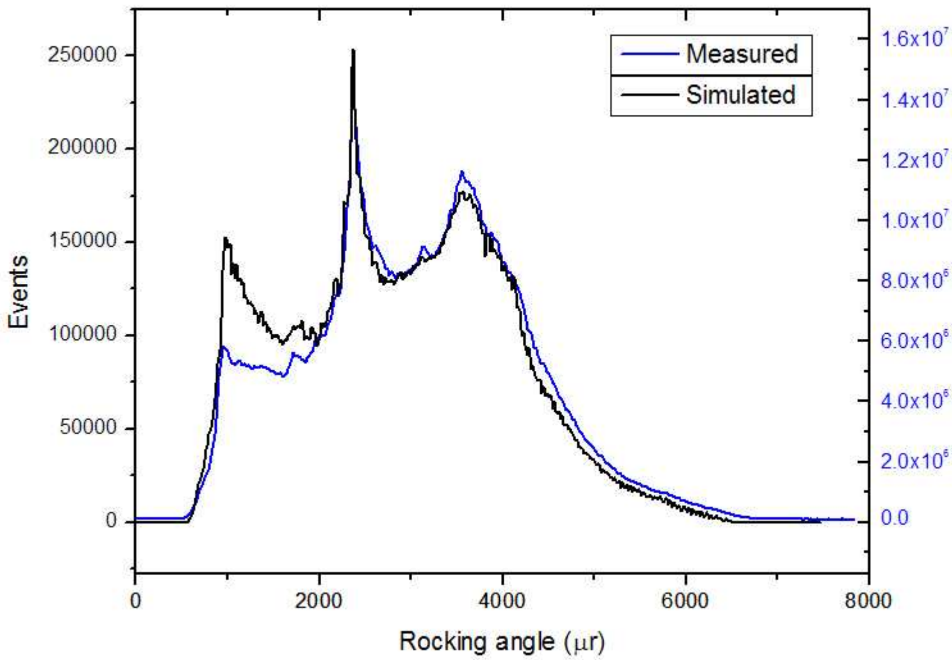

Figure 13. Diamond rocking curves, a) measured result, b) simulated result.

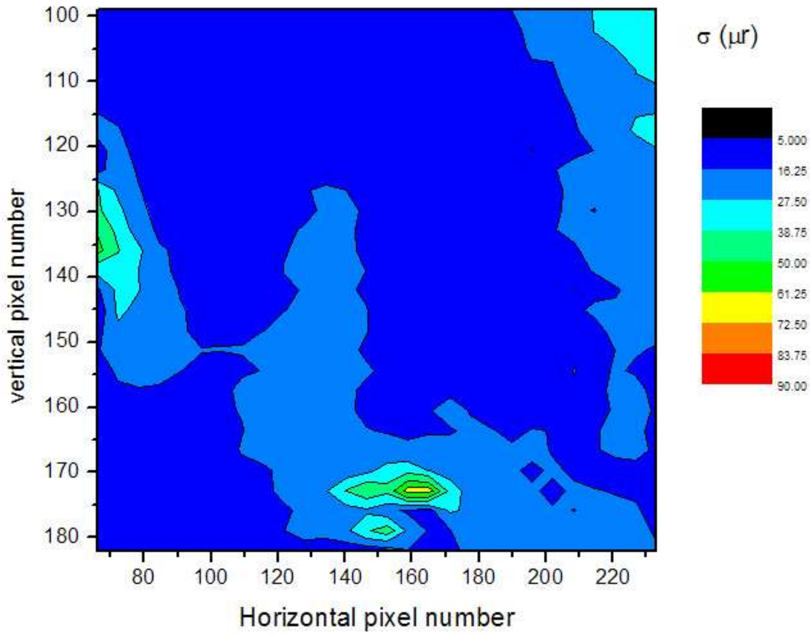

Figure 14. Simulated diamond 220 rocking curve width contour map.

From last year's rocking curve studies, we found that the 20 microns thick diamond is severely deformed by stress. The whole crystal has a very wide rocking curve peak and for a single pixel, the minimum rocking curve width could be as small as 30 μr and for different pixels the rocking curve peak positions are different. (If the crystal diffraction plane is all the same at different crystal locations, the measured rocking curve should have the same rocking curve peak position (if the d spacing is all the same for different positions)). By using the reconstructed crystal shape of the 20 microns thick diamond, the rocking curve for the whole crystal was simulated. In this simulation, the crystal is assumed to be perfect at all positions and the crystal orientations are different for different positions. In figure 13, the rocking curves for the 20 microns thick diamond were shown. It can be seen that the simulated rocking curve has the same featheures as the measured rocking curve. The difference between the simulated rocking curve and the measured rocking curve may derive from the crystal mosaic spread, where in the simulation it is assumed the whole crystal is perfect, while the real crystal mosaic spread values vary from position to postion. In figure 14, the simulated rocking cuve width contour is shown. It can be seen that although the whole crystal is assumed to be perfect, the simulated rocking curve width varys with the variation of positions. This phonomenon confirmed that the crystal curvature contribut significantly to the single pixel rocking curve width.

Conclusions

Simulation of the diamond crystal rocking curve was carried out by ray tracing method. The calculated results agree well with the measured diamond crystal rocking curve results. It was found that asymmetric monochromator can expand the beam spot size, but if there is no restrict collimation upstream of it, the large beam bandwidth caused by the large beam divergence will result in a large rocking curve width. Due to the excellent match between the silicon 331 and diamond 220 diffraction angles, silicon 331 asymmetric monochromator gives very narrow diamond 220 rocking curve width; hence it is well suited to be used for the diamond 220 rocking curve study. While a silicon 333 asymmetric monochromator generate rather broad rocking curve width due to the large beam bandwidth. A second monchromator can be used to reduce the beam bandwidth. Although the second monochromator affects the beam size, if the source vertical size is large enough, it is possible to get a large beam spot to measure the whole diamond crystal. The crystal curvature contribution to the rocking curve width for each pixel is investigated.

References.

[1] G. Yang. Hall D notes, GlueX Experiment Document 762-v1, 2007.