Effects of Diamond Crystal Imperfection on Coherent Bremsstrahlung

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Abstract

Coherent bremsstrahlung spectra from 3 thin diamond crystals with different crystal qualities have been measured. By using least squares fitting, theoretical calculations are matched to the experimental results. It is found that an extra incoherent background is needed in order to optimize the fitting. Bethe-Heitler theory gives the best description of the diamond incoherent part, and the calculated coherent spectrum needs about a 2% extra incoherent background. This means a better theory is required to give more accurate predictions. It has also been found that crystal defects and radiator temperature variations caused by electron beam heating do not have significant effects on the measured bremsstrahlung spectra. However, by comparing the bremsstrahlung spectra of different diamonds it was found that a diamond with a narrow rocking curve width has a sharper coherent bremsstrahlung peak edge than a diamond with a wide rocking curve width. A radiation damaged diamond shows evidence that it suffers from a macro stress which slightly deforms the diamond crystal, and causes a coherent peak shift.

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1 Introduction.

Due to its high Debye temperature and small lattice constant, a single diamond crystal is the most suitable radiator to generate coherent bremsstrahlung. In this process, a beam of high energy electrons strikes the crystal and a beam of γ-rays is emitted along the beam direction. The emitted photon beam consists of a coherent part and an incoherent part. By carefully selecting the electron incident angle with respect to a particular crystal plane, highly linearly polarized coherent photons can be obtained. This is very useful for studying many photon induced nuclear reactions. The characterization of linearly polarized coherent bremsstrahlung is described by many parameters, the most important of which are the electron beam divergence and energy spread, multiple scattering, and crystal quality. Timm[1] discussed theoretically the effects of all these parameters, while Lohmann [2] described the experimental effects of the parameters apart from crystal quality. Here, we present our results on the effects of crystal quality on the bremsstrahlung spectra. These investigate the effects of crystal quality on both the coherent part and the incoherent part.

1.1 Crystal imperfections.

Any diamond crystal contains certain defects. These can be point, line, planar defects, inclusions or complicated clusters of impurity atoms. These defects are usually generated during the diamond forming process due to an imperfect environment. In addition, there are two principal ways in which defects are generated after diamond formation. The first one is the plastic deformation created when the diamond crystal is subjected to high temperatures and high pressures while undergoing metamorphosis. The plastically deformed diamond contains a large number of line defects, which dramatically affect it's properties. The second one is radiation damage. Radiation of sufficiently high energy can displace atoms from their lattice positions, creating displacement damage. The primary defects caused by electron radiation are vacancy and interstitial and their complexes, and the defect density increases with increasing electron dose. Though diamond is believed to have very high radiation hardness, it has been found that after a certain dose of electron radiation, it is not suitable as a coherent bremsstrahlung radiator[1]. One of the most important consequence of electron radiation is that it causes serious strain or stress in the diamond crystal, which increases the crystal mosaic spread. In addition, a large concentration of defects causes serious disorder in the atomic distribution, which alters the static Debye-Waller factor[3].

1.2 Effects of crystal imperfections on the coherent bremsstrahlung spectrum.

Coherent bremsstrahlung occurs when one of the crystal reciprocal lattice vectors falls within the region of possible momentum transfer values defined by the momentum "pancake", which is derived from the kinematics of coherent bremsstrahlung[1]. By carefully selecting the incident angle of the electron beam with respect to the given crystal plane, we can let only one reciprocal lattice vector fall into the pancake in the energy region of interest. This will generate a single peak of coherent bremsstrahlung which has an upper limit edge. That upper limit follows the equation,

$$x_d = \frac{2E_0 q_l}{1 + 2E_0 q_l}$$

where q_l is the longitudinal component of the reciprocal lattice vector,ie along the incident beam direction. E_0 is electron beam energy and $x_d = k/E_0$, where k is the photon energy corresponding to the edge. When the diamond crystal has a large mosaic spread, there is a variation in the direction of a given reciprocal lattice vector throughout the crystal, and hence q_l will be slightly different for different electrons. A different q_l leads to a different x_d, and the averaged effect is that the edge of the coherent bremsstrahlung peak becomes broader and looses the sharp definition corresponding to a single q_l.

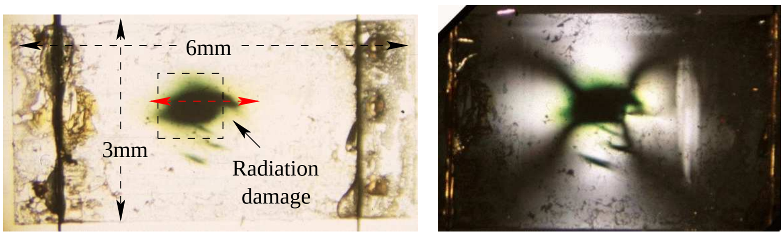
1.3 Effects of crystal imperfections on the incoherent bremsstrahlung spectrum.

Incoherent bremsstrahlung is caused by the thermal motion of atoms, and has a close relationship with the thermal Debye-Waller factor (f) [1], where $f = exp(-\sigma^2 q^2)$. σ^2 is the mean-square thermal displacement of the atoms, and q is the reciprocal lattice vector. σ^2 depends on the Debye temperature and the radiator temperature. The Debye temperature is believed to be largely unaffected by crystal imperfections, but the radiator temperature changes with changing beam intensity, beam spot size, crystal thickness, and crystal thermal conductivity[4]. Experimentally, the beam optics and the thickness of the crystal can be fixed, but the crystal thermal conductivity is not a constant, since it depends on the crystal quality and temperature[5,6]. Hence, crystal quality affects the thermal Debye-Waller factor, and subsequently the incoherent intensity.

Recent studies on the elastic scattering of particles in materials[3,7,8] have shown that the atomic disorder caused by defects has the same effect as the thermal motion of the atoms. A modified Debye-Waller factor $f_m = exp(-\sigma_m^2 q^2)$ has been introduced. σ_m^2 is the overall atomic disorder, which has a thermal part (σ_t^2) and a static part (σ_s^2). They are related by the equation $\sigma_m^2 = \sigma_t^2 + \sigma_s^2$. The thermal part (σ_t^2) is related to the amount of atomic displacement caused by thermal motion of the atoms, and the static part (σ_s^2) is related to the amount of atomic displacement caused by defects. The static part increases with an increase in defect density. Although the effect of static disorder on bremsstrahlung production has not been investigated until now, it has already been found that it has a significant influence on the Mossbauer effect [9] which is rather similar to coherent bremsstrahlung. Hence, we expect the static and thermal parts of the modified Debye-Waller factor to have similar effects on bremsstrahlung production.

2 Apparatus and experimental method.

2.1 Tagged bremsstrahlung.



(a) (b)

Figure 1: Petrographic microscopy of the radiation damaged diamond sample without (a) and with (b) crossed polaroids.

Three diamond crystals had been investigated in the research described in this report. For each, coherent bremsstrahlung spectra were obtained using

Table 1: A table listing the samples used in the present report

Sample	type	Thickness (μm)	Plane	Synthetic or Natural	FWHM (μradian)
Mainz	Ia	100	(001)	Synthetic	19–500
dBb	Ib	100	(001)	Synthetic	23
Gwugr	IIa	100	(001)	Synthetic	500

the MAMI-B microtron at Mainz. The diamond properties are shown in table 1. The Mainz diamond is a badly radiation damaged diamond. The damaged region is shown on Fig1. It is believed that about 10^{20} electrons have passed through the damaged region. The electron beam was passed through each diamond crystal and the energies of the residual electrons measured using the Glasgow tagged photon spectrometer[10]. The photon energy spectrum was obtained directly from the residual electron energy spectrum.The diamond wafers were aligned relative to the electron beam according to the technique developed by Livingston[11].

2.2 Rocking curves and mosaic spread.

The rocking curve of a sample is the variation in the reflected X-ray intensity as the sample is rotated relative to the incident beam to make its orientation pass through the Bragg condition. By rocking curve measurement, we can determine the crystal quality. Mosaic spread is a quantitative factor that describes the crystal quality, and it has a close relationship with the rocking curve width. According to the mosaic model[12], an imperfect crystal is believed to be composed of a large number of small mosaic blocks; within each block the distribution of the atoms is perfect, but for different blocks, the crystal planes have different orientations. Usually we assume the mosaic distribution has a Gaussian distribution. The mosaic spread(σ) is the square root of the standard variance of the orientation distribution. If we assume the rocking curve also has a Gaussian distribution,the mosaic spread can be estimated from the rocking curve half width; ie the $FWHM = 2.35 \times \sigma$ .The rocking curve measurements were carried out using the Synchrotron Radiation Source at Daresbury. For the diamonds dBb and Gwugr the measurements were performed at the geometrical centre of the diamonds, and for the radiation damaged diamond (Mainz) , the measurements were carried out along the red arrowed line shown in Fig 1a. Several measurement points are located in the radiation damaged region, and the others in an undamaged region.

2.3 Least squares simulation.

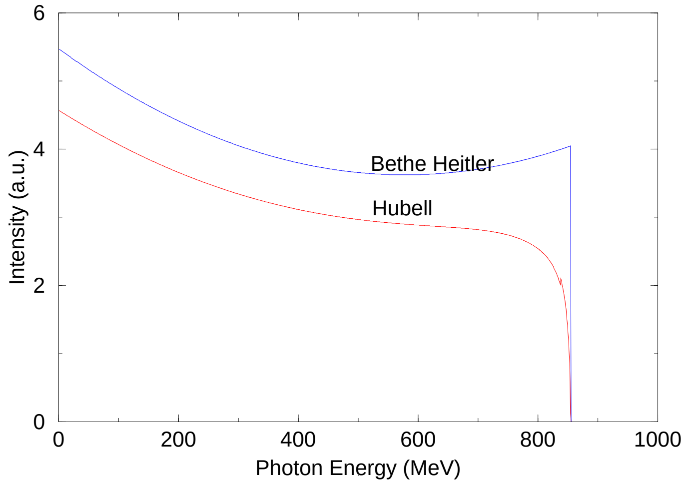


Figure 2: Bethe Heitler and Hubell calculations of the electron contribution to incoherent bremsstrahlung production for the same experimental parameters.

As we know, the bremsstrahlung from a crystal has a coherent part and an incoherent part. The incoherent part also contains a crystal contribution and an electron contribution. Natter[13] has developed a computer programme which calculates the bremsstrahlung from a diamond single crystal and an amorphous nickel radiator. Two different theoretical approaches (Bethe-Heitler and Hubell) are used to calculate the incoherent part. The different electron contributions to the incoherent part can be seen in Fig 2. In this report we will try to find which approach is better at fitting the measured spectra .

Another problem with the incoherent part is that it depends on the radiator temperature and the Debye-Waller factor, and it is not possible to measure the influence of these two factors independently. Our approach to find the best theoretical fit to an experimental bremsstrahlung spectrum from a diamond radiator is to add an adjustable extra incoherent component to the theoretical intensity and minimize X^2, where $X^2 = (I_{me} - (\alpha I_{dt} + \beta I_{nt}))^2$. I_{me} is the measured intensity of diamond bremsstrahlung, I_{dt} is the calculated theoretical intensity of diamond bremsstrahlung, and I_{nt} is the calculated theoretical amorphous intensity for nickel. α and β are two parameters, which are varied to minimize X^2, and hence find the best fit.

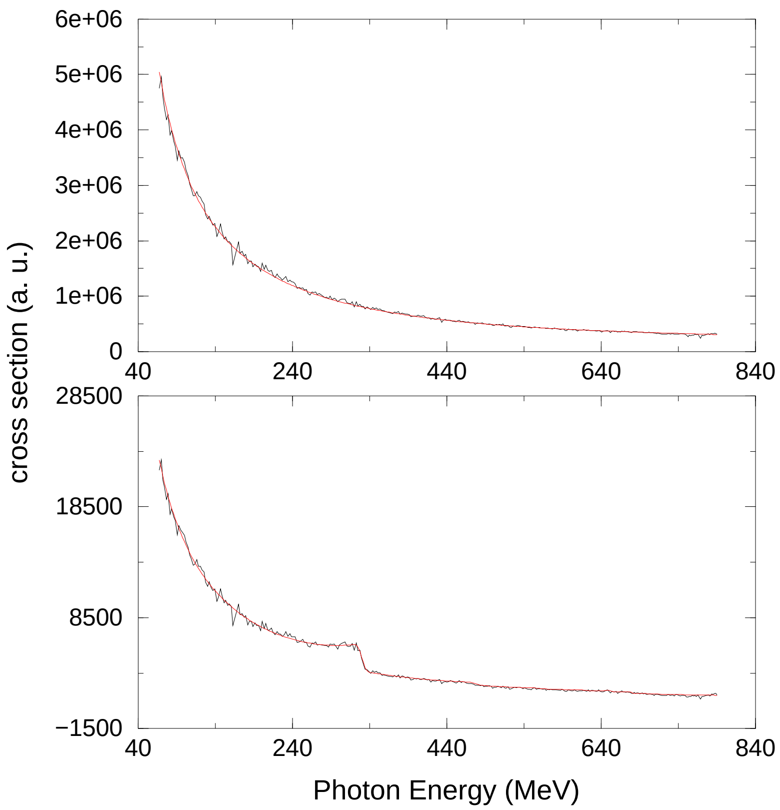


Figure 3: Comparison of measured data (black line) and the theoretical least squares fit (red line) for the absolute bremsstrahlung intensity for nickel (top) and diamond (bottom) .

Table 2: Least squares simulation results using B–H and Hubell theories: $\mu_s = \beta/\alpha$, with the subscript $s = BorH$. B represents B–H theory and H represents Hubell theory. For the Mainz diamond x is the position along the red arrowed line shown in Fig 1a. For dBb and Gwugr Φ_H is the goniometer rotation about the horizontal axis.

No.	Mainz		dBb		Gwugr	
	x (mm)	μ (%)	Φ_H (mr)	μ (%)	Φ_H (mr)	μ (%)
1	-1.5	2.4	9.74	1.8	14.8	3.2
2	-1.2	2.9	9.49	2.3	12.8	1.7
3	-0.9	3.4	9.23	2.4	10.8	3.4
4	-0.6	3.8	8.99	1.7	7.8	0.2
5	-0.3	2.6	8.74	1.9		
6	0	3.2	8.50	1.6		
7	0.3	4.3	8.24	0.5		
8	0.6	4.7	6.74	2.6		
9	0.9	3.5	4.24	1.8		
10	1.2	4.6				

3 Results.

It was found that, after introducing the extra incoherent background, the fitted theoretical results agreed well with the measured results. This can be seen from Fig.3. In Fig. 3, the black line is the experimental measurement and the red line is the theoretical fit.The fitted extra background values can be found in table 2 for different diamond crystals and test conditions. For the Bethe-Heitler theory, the values of the fitted extra incoherent background are in the range of (0-5)%, and for Hubell theory, the values are about two times larger. It was also found that for different diamonds, these extra incoherent backgrounds are slightly different. For the Mainz diamond, the coherent bremsstrahlung were taken at different points along a line going through the radiation damaged region, where the $x = 0mm$ point is located in the damage center. Although, in the damaged region, radiation damage caused many defects, as can be observed from the discoloration of the damage center and from the wide rocking curve widths, there is no significant change in the amount of extra background required between the damaged and the undamaged regions. This means the disorder caused by the radiation at the dose level and electron beam energy used has little effect on the incoherent bremsstrahlung spectrum. For the dBb and Gwugr diamonds, the measurements were carried out at a fixed position but at different electron incident angles. Because the change in angle is extremely small, we expect to obtain essentially the same results for different angles. Since the resulting extra background changes randomly with the angle setting, it seems the variations in the extra background are not coming from the crystal quality changing, but from experimental uncertainties.

Another factor that effects the bremsstrahlung background is the radiator temperature. The background increases with temperature, and we find the extra background can be accounted for by assuming the radiator temperature increasing to about 800 K. At present, the diamond temperature can not be measured directly during the bremsstrahlung measurements, but it is possible to estimate the upper limit of the temperature. In our experiments, the diamond radiator is glued to two vertical tungsten wires by an organic glue. Since a temperature higher than 500 K will destroy the glue, and the diamond has never separated from the wires, the radiator temperature is not very high. Theoretical predictions have also estimated that the radiator temperature does not exceed 400 K in normal conditions[14]. So it is unlikely the radiator temperature will influence the incoherent part of the bremsstrahlung significantly.

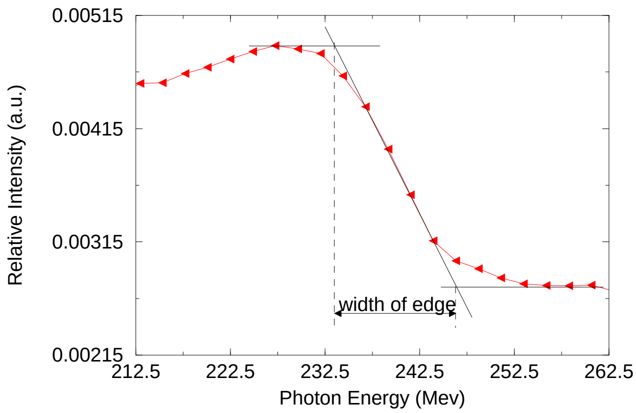


Figure 4: Definition of the width of the coherent peak edge.

Though crystal imperfections have little effect on the incoherent bremsstrahlung, we have observed some effects on the coherent part. We find that for

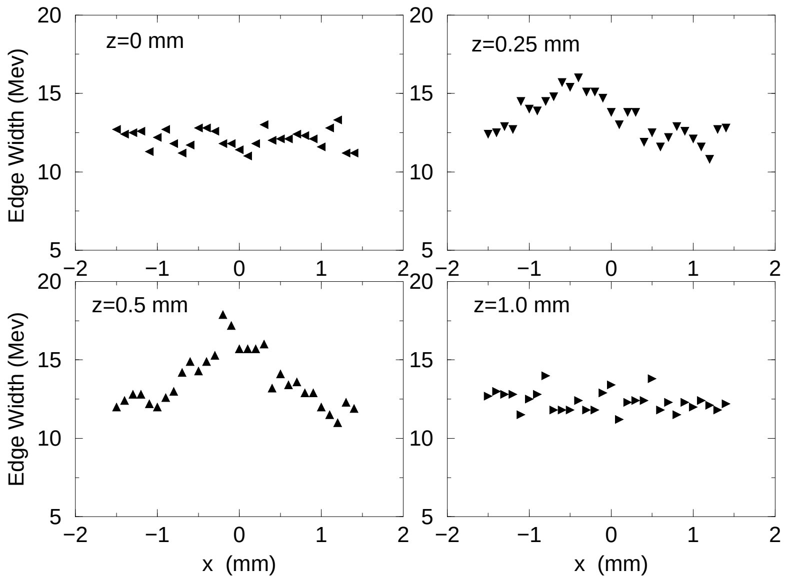


Figure 5: The variation of the width of the coherent edge of the Mainz diamond with x and z position. Referring to fig.1 the x-axis is horizontal and the z-axis vertical, with the origin at the damage center. When z=0.25mm and 0.5mm, the x scan goes through the damaged region.

a radiation damaged diamond (Mainz) and a plastically deformed diamond (Gwugr) the width of the coherent edge becomes broader. The way we define the coherent width of edge is illustrated in the Fig4. The triangular symbols describe the measured data points, the two straight lines parallel to the x axis go through the maximum and minimum of the coherent edge, and the third line defining the slope of the edge intersects the two horizontal lines. These two intersections define a line segment, the projection of which onto the x-axis is the width of the edge. For the Mainz diamond Fig5 gives the width of the edge as a function of x at different z coordinates. It is seen that in Fig5 b and c , the width changes with x, and reaches an maximum at about $x = 0mm$. However, in Fig5 a and d, the width of the edge is almost constant. The x scans at $z = 0.25mm$ and $0.5mm$ go through the radiation damaged region, whereas the z=1mm and 0mm scans are outwith the damaged region. From Fig 6, we find that the rocking curves of the badly damaged region are much broader than those far from the damage

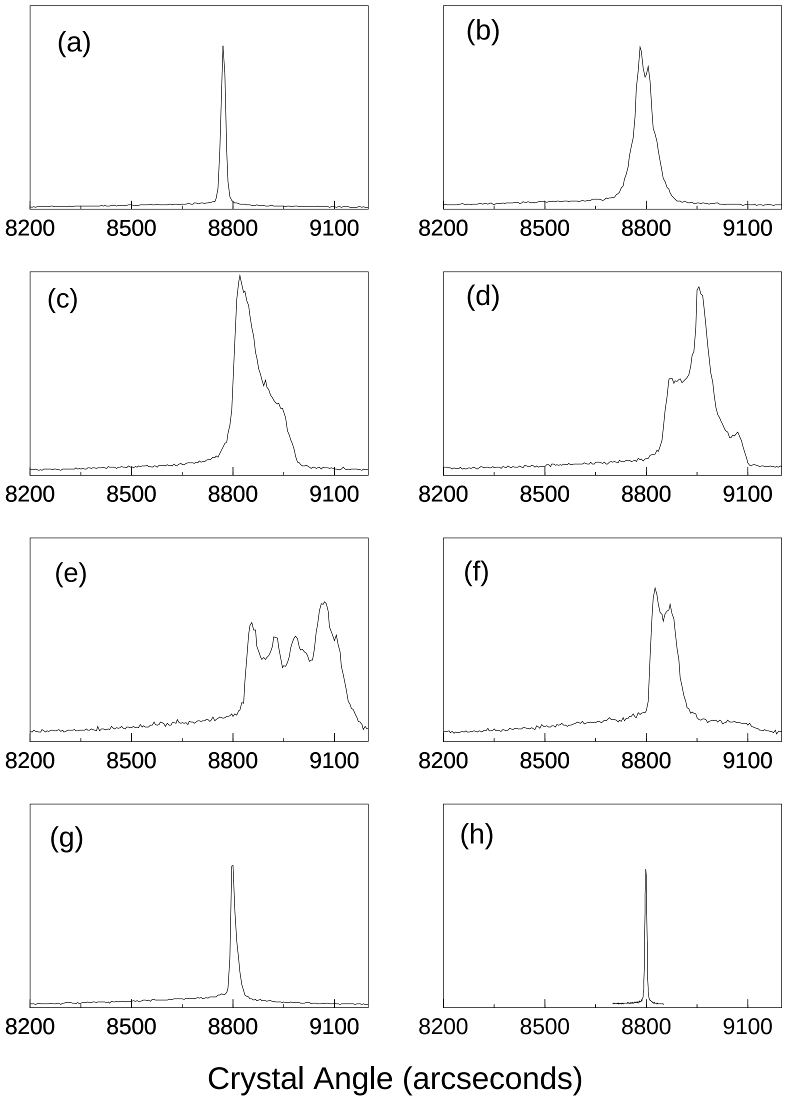


Figure 6: Rocking curves at different positions along a line going through the radiation damaged center. For a-h, each point has a distance from the damage center of: -0.75mm, -0.50mm, -0.25mm, -0.0mm, 0.25mm, 0.50mm, 0.75mm, 1.0mm

center. That means the damaged region has a much larger mosaic spread. From the rocking curves we estimate the mosaic spread of the damage center is about $0.2mr$, and far from the damage center, it is about $0.01mr$. It is clear that radiation damage results in a dramatic increase in the mosaic spread. Comparing with the results showed in Fig5, we find a large mosaic spread corresponds to a broader coherent bremsstrahlung peak edge, which is consistent with the prediction of Timm[1].

Because mosaic spread, multiple scattering and beam divergence have similar effects on the diamond coherent bremsstrahlung spectrum, we should take them all into account. The total effective angular spread(σ_{total}) is given by

$$\sigma^2_{total} = \sigma^2_{mosaic} + \sigma^2_{multiple} + \sigma^2_{beam}$$

where σ_{mosaic}, $\sigma_{multiple}$ and σ_{beam} refer to the mosaic spread, multiple scattering and beam divergence respectively. For the 855 MeV Mainz electron beam the bremsstrahlung characteristic angle $m_e c^2/E_0 = 0.6mr$,where m_e is the electron rest mass, and E_0 is the electron beam energy, and for a $100\mu m$ thick diamond, the r.m.s. multiple scattering angle is about $0.26mr$ [2]. The beam divergence is believed to be less than $0.1mr$ in our experiments, so the total effective angular spread is about $0.34mr$ for the damage center and $0.28mr$ away from the damaged region. For the Mainz beam energy the overall angular spread does not change dramatically even although the mosaic spread shows such a large difference between the damaged and undamaged regions.

But it should be remembered that the characteristic angle for a higher electron beam energy will become much smaller, and hence much more sensitive to the beam divergence, multiple scattering, and mosaic spread[1]. For example for 12 GeV, the characteristic angle is about $0.042mr$. Hence, if we use a beam divergence of $0.007mr$, which is the designed goal for hall D[14], and use a 20 μm thick diamond which has an r.m.s. multiple scattering angle of about $0.006mr$, then when the mosaic spread changes from $0.01mr$ to $0.2mr$, the overall angular spread will change from $0.014mr$ to $0.2mr$.

Another important consideration for the radiation damaged diamond crystal is, that not only is there a non-uniform strain caused by the defects, but there will also be a large uniform stress caused by a slight volume expansion resulting from the large number of defects in the diamond crystal. The volume expansion had already been observed by other authors studying radiation effects[15]. The petrographic microscopy of radiation damaged

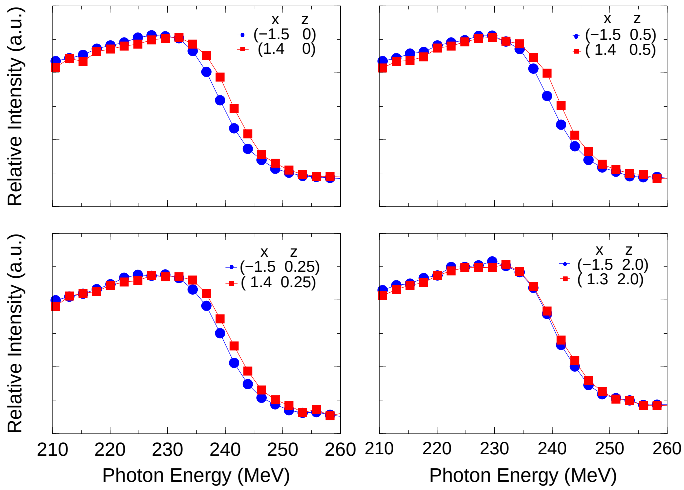


Figure 7: Relative intensity $(I^{coh} + I^{incoh})/I^{incoh}$ of bremsstrahlung spectra for the Mainz diamond at different positions. Referring to fig.1 the x-axis is horizontal and the z-axis vertical, with the origin at the damage center.

diamond shows a stress pattern like the stress caused by a large inclusion. It reveals a uniform strain field with 4-fold symmetry, as is shown in Fig 1. A diamond crystal suffering from such stress will contain certain macro deformations. This means an affected diamond crystal plane will not remain flat, but will become curved. So the crystal orientation of different parts will be different, which will lead to a coherent peak shift. This phenomenon is readily observed experimentally in Fig7. In Fig7, there are four diagrams, each containing two bremsstrahlung spectra at two different points. The coordinates of these points are shown on the right corner of each diagram. These spectra were taken using the same electron beam incident angle with respect to the diamond crystal plane, and we expect to obtain the same peak positions for each spectra. However, from Fig7 a, b and c, a difference between these two bremsstrahlung peak positions as large as 1 to 2 MeV is seen. That means the actual incident angle for each point is slightly different. So it is reasonable to believe that there is a different angular offset for each point. This observation indicates that the diamond is probably curved. For Fig7 d, the peak position difference is much smaller. These two points are far from the damage center, where the effect of the macro stress is smaller.

4 Conclusions.

In this report, we have discussed the effects of crystal imperfections on bremsstrahlung production. It has been found that the atomic disorder caused by defects and radiator temperature variations does not have a significant effect on the coherent bremsstrahlung spectra measured by the Glasgow tagger in Mainz, even though the diamond rocking curve widths were dramatically enlarged by radiation damage. Bethe-Heitler theory seems to give a better description of the diamond incoherent part, but since around 2% extra background is needed, a better theory is required to give more accurate predictions. It is also found that crystal imperfections cause the coherent edge width to become broader. For the radiation damaged diamond, a uniform strain caused by an associated volume expansion leads to a coherent bremsstrahlung edge shift. For a 12 GeV electron beam, a thin high quality diamond crystal with a small mosaic spread is essential. In particular, for a 20 micron diamond, if the mosaic spread changes by a factor of 20 from 0.01 to 0.2 mr, it is estimated the overall angular spread of the electrons will change by a factor of 15, from $0.014mr$ to $0.2mr$.

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