Lawrence Livermore Laboratory

CHANNELING AND COHERENT BREMSSTRAHLUNG EFFECTS
FOR RELATIVISTIC POSITRONS AND ELECTRONS

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March 22, 1976

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Prepared for U.S. Energy Research & Development Administration under contract No. W-7405-Eng-48.

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ABSTRACT

p. 1

I INTRODUCTION

p. 2

II CHANNELING OF RELATIVISTIC ELECTRONS
AND POSITRONS

p. 7

A. Theory

p. 7

B. Experiment

p. 16

C. Discussion of Data

p. 17

III COHERENT BREMSSTRAHLUNG

p. 40

A. Theory

p. 40

B. Experiment

p. 48

C. Discussion of Data

p. 51

IV CONCLUSIONS

p. 59

ACKNOWLEDGMENT

p. 61

REFERENCES

p. 62

APPENDICES

A. Silicon Lattice Structure

p. 65

B. Coherent Bremsstrahlung Computer Program

p. 73

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ABSTRACT :

Channeling of positrons in single crystals of silicon has been observed in transmission and scattering measurements for incident energies from 16 to 28 MeV. In addition, the spectral dependence upon crystal orientation of the forward coherent bremsstrahlung produced by beams of 28 MeV positrons and electrons incident upon a 5 μm thick single crystal of silicon was measured with a NaI photon spectrometer. Effects of channeling and perhaps of the non-validity of the first Born approximation were observed for beam directions near the $\langle 111 \rangle$ axis of the crystal, and coherent peaks near 0.5 MeV were observed for a compound interference direction, in agreement with first-order theoretical calculations.

I. INTRODUCTION

Channeling of relativistic positrons and coherently produced bremsstrahlung from both electrons and positrons in single crystals of silicon has been observed in transmission and scattering measurements for incident energies from 16 to 28 MeV. Beams from the Lawrence Livermore Laboratory linear accelerator were used in the study of the axial and planar channeling and the accompanying bremsstrahlung spectra from relativistic electrons and positrons impinging upon thin (5 to 53 μm) single silicon crystals. The resulting data indicate that the positrons channel in a classical manner, the electrons behave in a manner different from that observed at lower energies (see below), and either type of particle produces coherently generated bremsstrahlung when incident at a small angle with respect to a major direction in the crystal.

The concept of charged particle channeling deals with the multiple small angle scattering of charged particles in preferred directions by crystal lattice structure. An energetic charged particle impinging on a crystal structure within a calculable angle centered about a particular direction will be channeled along a string of atoms in that direction (axial channeling) or between planes of atoms parallel to that direction (planar channeling) by a succession of small angle scatterings which effectively steer the particle, preventing it from suffering any large angle scatterings due to close collisions with individual lattice atoms.

Channeling was predicted as early as 1912 by Stark and Wendt (1), but experimental difficulties prevented its detection. It was first observed and reported in 1960 by Davies (2) when experimental measurements of the range of ions in amorphous and crystalline solids were compared. The range profile in amorphous solids exhibited an approximately Gaussian form as expected from purely classical theory (3), whereas polycrystalline samples invariably exhibited a deeply penetrating tail. In 1963, Robinson and Oen (4) studied the classical penetration of ions in regular crystalline lattices using a high speed computer which predicted exceptionally long trajectories in preferred directions in the crystal lattice. Several experiments followed immediately which provided conclusive experimental evidence in support of the channeling phenomenon. Gemmell (3) has reviewed the theoretical and experimental studies of channeling reported on as of June 1973.

The original practical objective of studying relativistic positron channeling was to determine the degree of relative enhancement of the positron in-flight annihilation photon peak. It was reasoned that a majority of the positrons incident upon the single crystal annihilation target collinear with a string direction would be channeled. In such a case, only the unchanneled particles would suffer bremsstrahlung-producing scatterings, while a much greater fraction of the total beam positrons could undergo in-flight pair annihilation with the orbital electrons. Since channeling reduces the probability for large-angle scattering, the primary bremsstrahlung spectrum

intensity should be reduced with a relative increase in the nearly mono-energetic annihilation peak.

A preliminary experiment conducted in January 1969 (5) showed that channeling of relativistic positrons did occur and that bremsstrahlung was an orientation-dependent phenomenon also. The intensity of the unscattered-transmitted positrons increased as the incident particle beam was aligned with an atomic string direction in the crystal. The forward bremsstrahlung intensity decreased upon alignment as expected.

Section II describes a channeling experiment conducted in August 1969 that demonstrated the expected behavior for positrons. For both electrons and positrons there was an enhancement of the low-energy portion of the bremsstrahlung spectrum. However, the channeling effect for electrons was weak. Both axial and planar channeling of positrons were observed clearly for several silicon crystals. The data for electrons reflected an angular dependence upon the incident beam alignment which could not be explained from experiments conducted at lower energies (6). However, additional experiments (7,8) at energies comparable to our experiment showed the same type of channeling response as we observed (5). The enhancement of the low energy component of bremsstrahlung in the angular region of alignment of the beam with a principal direction of the periodic structure of the crystal suggested the possibility of coherently produced bremsstrahlung. This phenomenon results from the consideration of the periodicity of the reciprocal lattice allowing only those lattice recoil momenta which

satisfy the Bragg condition and momentum and energy conservation. This interference effect is maximized in experiments where the observed bremsstrahlung photons are restricted by suitable collimation to near the incident particle direction (see below).

In 1935 Williams (9) predicted that an interference effect due to the coherence in the successive interactions of an electron passing near a row of atoms could lead to deviations from the one-atom bremsstrahlung formula. He used the method of virtual quanta replacing the perturbing field of a relativistic charged particle with an equivalent pulse of radiation. The frame of reference selected is where the electron is at rest, and the Coulomb fields of the moving nuclei are represented by two pulses of virtual quanta. Bremsstrahlung is then viewed as the scattering of virtual quanta by the electron. When a relativistic electron passes through a crystal along a row of atoms, the virtual quanta of the Coulomb fields of the nuclei can interfere with one another. Consider two nuclei located on opposite sides of and equally near to the path of an extreme-relativistic electron ($v \sim c$). If their separation along the path of the electron is d , the electron, in its own frame of reference, receives two equal and opposite pulses with a time $d/\gamma c$ of each other. The frequencies of such a combined field must lie between $c\gamma/d$ and $\frac{mc^2}{h}$. So, for relativistic electrons, complete interference will result when $\frac{c\gamma}{d} \sim \frac{mc^2}{h}$ or $\gamma \sim \frac{mdc}{h}$. Now, if the second nucleus is on the same side of the path, the interference will result in

enhancing the radiative effect. It should be noted that the interference is always present, even at low values of γ , but is then limited to the lower frequency region.

In 1956, Überall (10) used the Born approximation and a simple cubic crystal lattice to analyze the interference effect. He developed formulae for the intensity change of the Bethe-Heitler (BH) cross section for bremsstrahlung due to interference effects. The formulae take into account electron screening and lattice vibrations. Several experiments (e.g. 11, 12, 13) verified the predicted enhancement and highlighted the structure resulting from the discrete nature of the reciprocal lattice. In 1963, Mozley and De Wire (14) pointed out that the coherent spectrum could be further modified by strong collimation of the emergent bremsstrahlung resulting in a line spectrum superimposed upon a reduced incoherent background.

In general, with few exceptions (15, 16), the experiments have been conducted at high energies ($\sim$ GeV) and Diambrini (17) has reviewed both theory and experiments as of 1968. In this paper, the question of positron and electron channeling effects and the generation of coherent bremsstrahlung at low relativistic energies is addressed. Specifically, the influence of channeling on coherent bremsstrahlung production is examined along with the dependence of coherent bremsstrahlung spectra on incident particle charge-sign and angle.

II. CHANNELING OF RELATIVISTIC ELECTRONS AND POSITRONS

The classical concept of charged particle channeling involves the multiple small angle scattering from collisions with the atoms in a string or plane of a single crystal lattice. In other words, the particles undergo many consecutive glancing collisions. In such a case, a continuum potential obtained by replacing the actual periodic potential by an average potential along a string or plane can be used as a good approximation.

The channeling experiment deals with relativistic electrons and positrons which can be treated classically, as will be shown. However, as has been observed in the field of electron microscopy, low energy (non-relativistic) electrons exhibit strong diffraction effects. This phenomena is known as Bloch-wave channeling, i.e. one or more Bloch waves are anomalously absorbed or transmitted in a single crystal. The multi-beam dynamical theory of electron diffraction has been discussed by Howie (18) and Nip and Kelly (19, 20, 21).

A. Theory

In some cases channeling effects seen in single crystals can be interpreted using either the classical (particle) or quantum mechanical (wave) theory of the phenomenology involved. The applicability of either treatment is determined by the characteristic wavelength and the angular divergence of the incident radiation being channeled. The de Broglie wavelength for the incident relativistic electrons is very small compared

to the lattice separation distances. Expressed in normalized units ($\hbar/2\pi=c=m=1$), the atomic string separation distance along a $\langle 110 \rangle$ direction in silicon is 1980. The de Broglie wavelengths for 16 to 28 MeV electrons varies from .19 to .11.

Crystal interference effects can be detected only if the beam divergence of the incident radiation is less than the associated Bragg angles. Of course, the beam divergence must always be less than the width of the channeling response function in order to observe any channeling effect at all. The wave theory of channeling is applicable when the beam divergence, $\Delta\theta$, is less than the width of the channeling response function, θ_0 , which, in turn, is much less than the Bragg angle, given by $2d \sin\theta_B = n\lambda$ ($\Delta\theta < \theta_0 < 0.001\theta_B$).

When the Bragg angle is much smaller than the beam divergence of the incident radiation, the classical theory should be adequate. In the experiments to be discussed, the maximum possible beam divergence was 3 milliradians and the actual divergence was smaller. The observed channeling response widths were smaller yet. Since the planar separation distances in the silicon lattice are on the order of 1000, the corresponding Bragg angle for the range of relativistic energies investigated is $\sim 3 \times 10^{-5}$ radians. Hence application of the classical particle theory seems appropriate in this case.

There are fundamental phase-space arguments which can be invoked to determine the validity of the classical treatment. The criterion for applicability is that the number of bound states in transverse phase-space has to be larger than unity.

The number of states can be estimated by

$$N_P = (2\pi h)^{-1} \int P(x) dx \quad \text{for planar case} \quad (1a)$$

$$N_A = (2\pi h)^{-2} \int \{P(r)\}^2 2\pi r dr \quad \text{for axial case} \quad (1b)$$

where $P(x)$ and $P(r)$ are distribution functions for atomic planes and atomic strings. Using suitable approximations (3) estimates of the number of states for positron and electrons are given by

$$N_P^+ = \{0.6(E + 0.511) Z^{2/3} N d_P^3\}^{1/2} \quad (2a)$$

$$N_P^- = \{0.06(E + 0.511) Z^{2/3} N d_P^3\}^{1/2} \quad (2b)$$

$$N_A^+ = 0.62 (E + 0.511) Z (N d_S^2 a_0)^{-1} \quad (2c)$$

$$N_A^- = 0.063 (E + 0.511) Z (N d_S^2 a_0)^{-1} \quad (2d)$$

where E is particle energy in MeV, Z the atomic number of the crystal atom, N the number of atoms per unit volume, d_P is the planar separation distance, d_S is the string separation distance and a_0 is the Bohr radius.

In the present experiment, the values for Eqs. 2a, b, c, d are as follows

	16 MeV	28 MeV
N_P^+	4.5	5.9
N_P^-	1.4	1.9
N_A^+	244.0	421.0
N_A^-	24.8	42.8

From these numbers, we see that the classical particle theory is adequate to interpret the experimental results for axial channeling but questionable for planar channeling.

In 1965, Lindhard (22) formulated a comprehensive theory of directional effects for energetic charged particles in crystal lattices. The theory considers that the path of a particle channeled by a crystal lattice is primarily determined by the deflections due to the screened Coulomb scattering of a particle as it passes close to or through an atom. The theory is restricted to small-angle deflections from successive atoms in strings or planes such that the process can be considered as a scattering from a continuous string or planar transverse potential barrier. Charged particles incident at small angles along strings of atoms or between planes of atoms will be channeled along those strings or planes, if their transverse kinetic energy is less than the respective transverse potential barriers.

In the continuum string approximation, the potential due to a row of atoms is considered to be uniformly smeared out along the row. In Lindhard's theory, the continuum approximation is valid if the angle of incidence of the particle upon a row is less than Ψ_1 , where

$$\Psi_1 \equiv (2Z_1 Z_2 e^2 / d_s E)^{1/2} \approx 0.307 (Z_1 Z_2 / d_s E)^{1/2} \quad (3)$$

expressed in degrees and E is the energy of the incident particle. Ψ_1 is not the quantity actually limiting the channeling effect. The critical angle of incidence Ψ_c beyond which the distance of closest approach becomes less than the critical distance r_c for proper axial channeling is given by

$$\Psi_c = F_{RS} (r_c / a_{TF}) \Psi_1 \quad (4)$$

The quantity $\Psi_{1/2}$ is defined as half of the angle at the half minimum of the channeling dip response function. It is related to Ψ_C as follows (23)

$$\Psi_{1/2} = 0.8 \Psi_C = 0.8 F_{RS} (1.2\mu/a_{TF}) \Psi_1 . \quad (5)$$

The static-row continuum potential function F_{RS} (24) is plotted in Figure 1. The thermal vibration amplitude, μ , is given by the following relation based upon the Debye approximation for thermal lattice vibrations

$$\mu = 12.1 \{ \{ \Phi(\chi) / \chi + 1/4 \} / M_C \Theta \}^{1/2} \text{ \AA} \quad (6)$$

where

$$\chi \equiv \Theta/T$$

$$\Theta \equiv \text{Debye temperature } (^{\circ}\text{K})$$

$$T \equiv \text{Crystal temperature } (^{\circ}\text{K})$$

$$\Phi(\chi) \equiv \text{Debye function (plotted in Figure 2)}$$

$$M_C \equiv \text{Atomic weight of crystal atoms (amu)}$$

and a_{TF} is the Thomas-Fermi screening radius

$$a_{TF} = 0.4865 Z^{-1/3} \text{ \AA} .$$

A similar expression is developed for planar channeling

$$\Psi_{1/2} = 0.72 F_{PS} (1.6\mu/a_{TF}, d_p/a_{TF}) \Psi_P \quad (7)$$

and

$$\Psi_P \approx 0.545 (nZ_1Z_2a_{TF}/E)^{1/2} \quad (\text{degrees}) \quad (8)$$

where F_{PS} is plotted in Figure 3, d_p is the planar separation distance, and n is atomic density in planes $\{\text{atoms}/(\text{\AA})^2\}$.

The equations for the half angle are modified for the relativistic case by replacing the energy of the incident particle E by $1/2 pv$ where p is the relativistic momentum.

The calculated half angle for axial channeling in the

Fig. 1. Graph of the function $F_{RS}(\xi)$.

Fig. 2. Graph of the Debye function $\phi(x)$.

Fig. 3. Graph of the function $F_{PS}(\xi, \eta)$.

Fig. 4. Calculated half-angle $\psi_{1/2}$ for axial channeling, $\langle 111 \rangle$ and $\langle 110 \rangle$, and planar channeling, (110) and (112) .

$\langle 111 \rangle$ and $\langle 110 \rangle$ directions of the silicon lattice is plotted as a function of energy in Figure 4. Also included are the half angles for planar channeling between (110) and (112) planes of the silicon lattice.

B. Experiment

The channeling experiments were designed to investigate the channeling response by measuring the intensities of charged particles and photons transmitted through various collimators as a function of the angle between the incident beam and either the $\langle 111 \rangle$ or $\langle 110 \rangle$ directions of single crystals of silicon. Monoenergetic ($\Delta E/E \leq 1\%$) positron and electron beams were obtained from the Livermore electron-positron linear accelerator. The particles impinged upon thin (5 - to 53 - μm) silicon crystals mounted on a goniometer capable of sweeping the crystal through a two-dimensional angular range in 0.04 - mrad steps. A plastic scintillator was suitably collimated to allow separate observation of forward-transmitted particles, and of particles scattered into the angular ranges 0.5 to 0.6 and 0.9 to 1.0 deg with respect to the incident beam. A thin-walled transmission ionization chamber filled to 0.5 atm of xenon gas was used to observe the forward bremsstrahlung. In the bremsstrahlung measurements, a magnet which followed the crystal target swept transmitted particles away from the detector. The maximum angular divergence of the beam was determined by the use of suitable collimation systems. For particle observations, the beam collimation consisted of two 1/8-in.-diameter aluminum collimators placed 20 feet apart, with

no focusing elements between them. For the bremsstrahlung observations, 3/8-in.-diameter carbon collimators were employed. The 3/8-in. system provided a maximum beam divergence of 3 mrad, of the same order as the expected half angle for channeling. Careful tuning of quadrupole magnets in the beam transport system appeared to result in beam divergences considerably smaller than this value, since the positron transmission measurements performed with either set of collimators yielded essentially the same channel widths.

C. Discussion of Data

Curves representative of the main features of the data are shown in Figure 5, where the various measured intensities are plotted as a function of θ , the angle between the incident beam and the crystal direction. In all cases in the data for positrons, channeling produces a narrow structure in the curves, centered about $\theta = 0$. This is illustrated in Figure 5a for scattered 20-MeV positrons (scattered into the angular range 0.9 to 1.0 degrees with respect to the beam), for the $\langle 111 \rangle$ direction of a 42 μm crystal. Figure 5b represents the same measurement for electrons, and a similar though much less prominent narrow structure appears. Both curves show other broader structure. Curves for forward-transmitted ($\theta = 0$) particles have complementary shapes, as expected.

The particle data include measurements of the channeling of 16 to 28 MeV positrons in silicon single crystals. In Figures 6 through 10, the observed positron half angles ($\Psi_{1/2}$)

Fig. 5. Typical scattering response for positrons and electrons. (a). Scattering of 20-MeV positrons into an angular range of 0.9 - 1.0° with respect to the beam. (b) Same case for electrons. Data are for a $42\text{-}\mu\text{m}$ Si crystal, with θ the angle between the $\langle 111 \rangle$ crystallographic direction and the beam axis. Curves are normalized to equivalent off-channel values.

Fig. 6. Measured half-angles for positron channeling in the 5- μ m Si crystal. Half-angles measured by the 0.5-0.6° annular collimator are indicated by circles; those measured by the 3/16-inch-diameter direct transmission collimator, by squares. The $\langle 111 \rangle$ calculated half-angle is shown by the solid line for comparison.

Fig. 7. Measured half-angles for positron channeling in the 10- μ m Si crystal. Half-angles measured by the 0.5-0.6° annular collimator are indicated by circles; those measured by the 3/16-inch-diameter direct transmission collimator, by squares. The $\langle 111 \rangle$ calculated half-angle is shown by the solid line for comparison.

Fig. 8. Measured half-angles for positron channeling in the 19- μm Si crystal. Half-angles measured by the 0.5-0.6° annular collimator are indicated by circles; those measured by the 3/16-inch-diameter direct transmission collimator, by squares. The $\langle 111 \rangle$ calculated half-angle is shown by the solid line for comparison.

Fig. 9. Measured half-angles for positron channeling in the 42- μm Si crystal. Half-angles measured by the 0.9-1.0° annular collimator are indicated by the triangles; those measured by the 0.5-0.6° annular collimator, by circles; those measured by the 7/8-inch-diameter direct transmission collimator, by squares. The $\langle 111 \rangle$ calculated half-angle is shown for comparison.

Fig. 10. Measured half-angles for positron channeling in the 53- μm Si crystal. Half-angles measured by the 0.9-1.0° annular collimator are indicated by triangles; those measured by the 0.5-0.6° annular collimator, by circles; those measured by the 3/16-inch-diameter direct transmission collimator, by squares. The $\langle 110 \rangle$ calculated half-angle is shown for comparison.

as measured with different collimators in front of the detector are given as functions of energy for the various crystals investigated. The channeling response curves were determined by measuring the intensities of particles transmitted through the various collimators as a function of the angle between the incident beam and either the $\langle 110 \rangle$ or the $\langle 111 \rangle$ crystallographic direction.

The energy dependence of the axial channeling half angle for the unscattered transmitted positrons follows the $E^{-1/2}$ slope predicted by the Lindhard classical theory. Also, the half angle for scattered positrons as measured by the annular collimators ($0.5 - 0.6^\circ$ and $0.9 - 1.0^\circ$) generally shows an $E^{-1/2}$ dependence with the exception of low energy and thick crystals: Figure 8, 16 MeV, $0.5 - 0.6^\circ$, 19 μm ; Figures 9 and 10, 16 MeV, $0.9 - 1.0^\circ$, 42 μm and 53 μm , and especially (Figure 10) $0.5 - 0.6^\circ$, 53 μm . However, the magnitudes of the angles lie below the theoretical values. The standard deviations of the measurements are very small (± 0.03 mrad), on the order of size of the symbols representing the data points.

For narrow direct collimators, the effect of multiple scattering should be less than that for scattered particle collimators. This is because the multiple scattering distributions are broad with respect to the direct collimator aperture. Hence, a loss in signal from the multiple scattering distribution due to channeling will not compensate for the dramatic increase from unscattered (channeled) particles. This is

Fig. 11. Maximum/random intensity ratios. The ratio of the intensity of the maximum at the on-channel position to the intensity at a random off-channel position is plotted against energy for the 7/8-inch collimator (10- and 42- μm Si) and the 3/16-inch collimator (5-, 10-, and 19- μm Si).

shown in Figure 11 where the maximum/random intensity ratios are plotted as a function of energy for several crystals. Note the 10 μm crystal, 3/16-in. and 7/8-in. collimator data showing the decrease in intensity ratios for the larger aperture collimator which allows multiple scattering distribution losses to compensate the channeled particle signal gain. This is borne out by the calculated distribution in Figure 12 which shows the multiple scattering distribution is not significant beyond the 7/8-in. (0.54°) aperture except at the lower incident particle energy. As incident energy decreases, the distribution spreads beyond the 7/8-in. aperture, compensating losses are reduced, and the intensity ratio increases. The 42 μm crystal, on the other hand, has a multiple scattering distribution with a significant component beyond the 0.54° range which under channeling conditions results in higher 7/8-in. maximum/random intensity ratios.

In the case of the annular collimators, the channeling response is being sampled from the shoulders of the multiple scattering distribution. They are sensitive to only the loss in scattered particle signal due to channeling. The channeling response is modified by the multiple scattering distribution as shown in Figure 13. Note the 42 μm crystal, $0.5^\circ - 0.6^\circ$ and $0.9^\circ - 1.0^\circ$ annular collimator data showing the improved minimum/random intensity ratio for the larger angle of scattering where the multiple scattering component is lower. Also, the minimum/random intensity increases with energy as

Fig. 12. Multiple scattering distributions. Angular distributions of multiply scattered positrons are calculated for the 10- and 42- μm Si crystals at both 16 and 28 MeV. The 0.54° range corresponds to the 7/8-inch-diameter aperture.

Fig. 13. Minimum/random intensity ratios. The ratio of the intensity of the minimum at the on-channel position to the intensity at a random off-channel position is plotted against energy for the 0.9-1.0° annular collimator (42- μm Si) and the 0.5-0.6° annular collimator (19- and 42- μm Si).

the multiple scattering decreases.

In both Figures 11 and 13, the data for the 19 μm crystal shows its superior channeling properties and supports the arguments above on the influence of multiple scattering on the observed channeling response. The 19 μm crystal exhibited the highest maximum/random intensity ratios for the unscattered-transmitted particle channeling response. Also, the 19 μm crystal minimum/random intensity ratios for scattered particles were the lowest observed with the $0.5^\circ - 0.6^\circ$ annular collimator. The relatively inferior channeling properties of the 10 μm and 5 μm crystals are attributed to warping after mounting the ultra-thin crystals in the goniometer.

It is apparent that multiple scattering, not considered in the theory, is significantly affecting the particle channeling response. It tends to mask the true features of the particle channeling response. In addition to the above arguments, examination of the data in the form shown in Figure 5 reveals that the shoulder width and enhancement (peak above random) increased with energy, that is with decreasing multiple scattering distributions. It is reasonable to assign the strange response for low energy and thick crystals (noted above) to multiple scattering effects. However, from the data available, it cannot be demonstrated that multiple scattering is the reason for all the experimental data being consistently below the theoretical values.

The channeling process effectively steers the particles

along crystallographic directions when the beam is incident within the critical angle of a principal string. This effect was observed when the critical angle as measured by the various direct detector collimators ($7/8"$, $3/16"$, $1/8"$, and $1/16"$) decreased with decreasing collimator aperture. From these data, the actual beam divergence is estimated to be approximately $3'$. This is further supported by Table I which shows the measured half angle for both $1/8$ -in. and $3/8$ -in. beam collimators.

Positron channeling can be used as an orientation technique by mapping the major planes of the crystal as shown in Figure 14. This planar map was constructed from large angle (10°) scans made using the $0.5 - 0.6^\circ$ annular detector collimator with 28 MeV positrons incident upon the $5 \mu\text{m}$ crystal. The stereogram of the crystallographic direction $\langle 111 \rangle$ shown in Figure 15 was used to interpret Figure 14. The energy dependence of the planar channeling half angle is given in Figure 16. These values are corrected for the angle between the scan direction and the planes involved. For the perpendicular (112) case and the moderately oblique (110) cases at 60° , there is good agreement with the $E^{-1/2}$ dependence predicted by Lindhard for planar channeling. The disagreement as to magnitude may be due to the breakdown of the classical approximation (see above).

The electron particle data do not agree with expectations based on earlier electron-channeling work done at lower

TABLE 1

Dependence of String Channeling Critical Angle On Incident Beam Collimation

Detector Collimation			Measured Half Angles	
Collimator	Energy	Crystal	1/8" Beam Collimation	3/8" Beam Collimation
3/16"	28 MeV	53 μm	4.7'	4.8'
0.5-0.6 deg	28 MeV	53 μm	6.5'	6.6'
0.9-1.0 deg	28 MeV	53 μm	6.3'	7.3'
0.5-1.0 deg	28 MeV	53 μm	6.3'	6.7'

Fig. 14. Planar channeling map of the 5- μ m Si crystal. Long range scans form the data set which allows the mapping of major planes intersecting the principal crystal direction $\langle 111 \rangle$. This mapping technique was used to accurately orient the crystal in the coherent bremsstrahlung experiment.

MUB-2162

Fig. 15. Stereogram of the $\langle 111 \rangle$ crystallographic direction.

Fig. 16. Measured half-angles for positron planar channeling in the 5- μ m Si crystal. The measured values were corrected for the angle between the scan direction and the planes involved. Half-angles for (110) planes are indicated by crosses; those for (112) planes, by circles. The calculated half-angles for planar channeling are shown for comparison.

energies (6). However, the response function does agree with results at comparable energies [(7), (8)], where broad shoulders and a central dip were observed for electron channeling in single crystals of MgO. Although none of the scattered-electron response curves had strong enough central dips to accurately measure a half angle, the widths of the shoulders tracked very well with the positron data. Also, the shoulder-peak separation distance follows an $E^{-1/2}$ energy dependence as shown in Figure 17 for the 42 μm silicon crystal.

The bremsstrahlung data for both positrons and electrons show several interesting features. The upper curves in Figures 18 and 19 correspond to unfiltered bremsstrahlung detected by the ionization chamber. The positron data show the characteristic channeling dip; this was expected since bremsstrahlung production is a small-impact-parameter phenomenon. In addition, curves for both positrons and electrons show a broad structure rising above the off-channel values. When a 1/16-in. lead absorber was placed between the target and the ionization chamber the broad structure was essentially eliminated, indicating that it results from low-energy photons ($E_\gamma < 1 \text{ MeV}$). The narrow channeling dip for positrons is still seen with a 1/2-in. lead absorber, as shown in Figure 18 b; the high-energy portion ($> 1 \text{ MeV}$) of the bremsstrahlung spectrum is thus clearly influenced by the channeling phenomenon.

For a given bombarding energy and crystal, the broad structure associated with low-energy photons is similar in

Fig. 17. Measured shoulder peak-to-peak distance for electron channeling response in the 42- μm Si crystal for the 0.9-1.0° annular collimator. The $E^{-1/2}$ curve fits the first three points. The 28-MeV data point cannot be considered reliable because the response curve was not symmetric.

Fig. 18. Typical forward bremsstrahlung response for positrons.

(a) Forward bremsstrahlung detected by the ionization chamber, for 28-MeV positrons incident on a 53- μm Si crystal; θ is the angle between the beam axis and the $\langle 110 \rangle$ crystallographic direction. (b) Similar data, but with a 1/2-inch lead absorber between the crystal and the detector. Curves are normalized to equal off-channel values.

Fig. 19. Typical forward bremsstrahlung response for electrons.

(a) Forward bremsstrahlung detected by the ionization chamber, for 28-MeV electrons incident on a 53- μm Si crystal; θ is the angle between the beam axis and the $\langle 110 \rangle$ crystallographic direction. (b) Similar data, but with a 1/2-inch lead absorber between the crystal and the detector. Curves are normalized to equal off-channel values.

width to the broad structure seen in the particle-scattering experiments. This, together with the absence of residual broad structure in the curves for filtered bremsstrahlung suggests that these effects might be related. In the case of particle data for positrons, however, one could be observing the "shoulders" that normally are seen in channeling measurements and that are attributed to an increased probability for small-impact-parameter events. The shoulders are more prominent and narrower for higher incident particle energies, consistent with this interpretation. However, this type of interaction normally would not be expected to result in preferential production of low-energy bremsstrahlung photons. The appearance of the low-energy bremsstrahlung structure in the region of alignment of the beam with the periodic structure of the crystal suggests strongly the presence of coherently produced bremsstrahlung.

III. COHERENT BREMSSTRAHLUNG

The term coherent bremsstrahlung refers to the nature of the interaction between the charged particle and several atomic scattering centers in a row. The greater the number of atoms coherently generating the photon, the greater will be the enhancement of photons of that energy above the incoherent background. While the energy and angle of incidence of the charged particle generally determine the degree of enhancement, the reciprocal lattice geometry of the crystal primarily controls the energy at which photons will be enhanced.

A. Theory

The conventional theoretical treatment of coherent bremsstrahlung in single crystals is based upon the Born approximation (25, 26, 10, 17) and computer programs following that approach are used widely to predict photon spectra at high relativistic energies (27, 28, 29). The effects of photon collimation and multiple scattering are included in the calculations (Figure 20). However, the relative contribution of the second Born approximation becomes comparable to the contribution from the first for very small angles of incidence (30). This should result in an increase in the coherent bremsstrahlung intensity for positrons and a decrease for electrons. Additionally, channeling of relativistic positrons and electrons (5, 7, 8, 31) may affect the phenomenon. This has not been included in any theory to date. Axial channeling of positrons tends to keep the particles remote from the strings,

Fig. 20. Calculated coherent bremsstrahlung spectra. Intensity as a function of relative energy $x = k/\gamma$ for 28-MeV beam incident along a (110) plane, 50.5 minutes of arc from the $\langle 111 \rangle$ direction. The solid curve is based simply on the Born approximation (see Appendix B), while the dashed curve takes into account both collimation and multiple scattering in addition.

thereby reducing the probability of close encounters resulting in coherent bremsstrahlung. Electron channeling, on the other hand, increases the probability for close encounter interactions.

The validity of the Born approximation for the treatment of coherent bremsstrahlung has been discussed by several authors (25, 10, 32, 33, 30). In general, the Born approximation begins to fail for high atomic numbers, photon energies near the high frequency limit, and low incident electron energy. Schiff (32) pointed out that even for small Z the phase change of a wave function of an electron passing through a crystal can be very large. Hence Bloch wave functions are more appropriate than plane wave functions when treating coherent bremsstrahlung. Ferretti (25, 33) predicted that, for unitarity reasons, at very high energy, the Born approximation has to break down completely. He later (34) proposed a method for calculating coherent bremsstrahlung which is valid when the energy of the photon is very small compared to the incident particle energy. Unfortunately, the treatment is valid for positrons only. Akhiezer et al (30) show that at small angles of incidence the kinematical restrictions imposed by the allowed crystal recoil momenta lead to an increased relative contribution from the second Born approximation. Since that term is first order in Z , the contribution represents a potential means for discriminating between positron and electron coherent bremsstrahlung.

The relative contribution of the second Born approximation becomes appreciable at low relativistic energies. For 28 MeV

positrons incident at 1° from a major axis of a single crystal of silicon, the second approximation has a relative contribution of

$$\frac{Z\hat{\alpha}}{\gamma a_{TF}\theta^2} \sim \frac{(14)}{(55.8)} \frac{(0.0072)}{(50) (.0175)^2} = .12$$

where $\hat{\alpha}$ is the fine structure constant and γ is the incident particle angle. This effect may be observable. However, channeling may also affect the coherent bremsstrahlung production process. It might be useful therefore to select a random, asymmetric angle of incidence for the positron and electron beams so that channeling effects are eliminated. While an exact treatment of the intensity of coherent bremsstrahlung is lacking, certain qualitative features such as the energy of the peaks can be easily interpreted in terms of the kinematical limitations introduced by the reciprocal lattice. The energy of the peaks can be determined from the following approximate formula ($k \ll \gamma$, $\gamma \gg 1$)

$$\frac{k}{\gamma} \equiv X \approx \frac{2\gamma q_1 - q_2^2}{1 + 2\gamma q_1} \quad (9)$$

where k is the energy of the photon, γ is the energy of the incident particle, q_1 is the longitudinal momentum transferred to the crystal, and q_2 is the transverse momentum transferred to the crystal.

The transverse momentum term in this equation produces the curvature of the "momentum pancake" (10) so prominent at lower energies. It also results in the appearance of fine structure energy peaks superimposed on a large broad peak representing a row of reciprocal lattice points compounding

their contribution to the coherent bremsstrahlung. The fine structure results from pairs of reciprocal lattice points with equivalent q_2 on a row of lattice points all with the same q_1 . Such a condition results from the symmetry obtained when the particle beam is incident at a small angle with respect to any major axis along any major plane. It is obvious that beam divergence and multiple scattering will determine whether it will be possible to resolve such structure. Increasing the incident energy is not useful (in this regard) since the fine structure coalesces to a single peak representative of a "flat momentum pancake." This effect must be investigated at lower energies with small beam divergences and ultra-thin crystals. The effective beam divergence ϕ_{eff} is a function of collimation (measured by ϕ_b) and multiple scattering (measured by ϕ_{ms}), i.e.

$$\phi_{\text{eff}} = (\phi_b^2 + \phi_{\text{ms}}^2)^{1/2} \quad (10)$$

so that for a collinear beam $\phi_{\text{eff}} \propto t^{1/2}/\gamma$ where t is the crystal thickness. Yet, the curvature which determines the fine structure separation ΔE_{fs} varies as γ^{-1} , hence the experimental resolution of the fine structure $\Delta E_{\text{fs}}/\phi_{\text{eff}}$ is proportional to $t^{-1/2}$.

Photon collimation or so-called second collimation (35) causes the coherent bremsstrahlung peaks to become narrower, approaching line spectra as the collimator angles are reduced. Additionally, this reduces the incoherent part, thereby improving the signal to noise level. However, for low

relativistic energies, where curvature becomes significant, the net result will be to separate the fine structure into individual lines (neglecting beam divergence and multiple scattering).

Thus, for positrons and electrons incident at small angles with respect to major directions in single crystals, we should expect competing trends from channeling and the second Born approximation. As the angle of incidence is decreased, the intensity of coherent bremsstrahlung will increase for positrons until channeling becomes significant. Axial channeling half angles for silicon single crystals are on the order of two milliradians for incident particle beams with energies in the tens of MeV. It is reasonable for relatively thin crystals, 5 to 50 μm , to exhibit strong channeling response in particle beams with divergences of about one milliradian. Once the particle beam is incident within the angular range for channeling, a strong reduction for close encounter interactions should result for positrons. However, electron channeling keeps the particle near the atomic string, thereby, increasing that particle's probability of undergoing close encounter interactions. It is also worth noting that electrons channel in an oscillatory manner around one atomic string making them very susceptible to thermal and zero point motion while positrons channel relatively long distances unperturbed by lattice motion.

Fig. 21. Experimental apparatus. The high-current electron beam from the first accelerator section (1) strikes the 0.25-cm-thick tungsten positron converter (2), producing in turn bremsstrahlung and positron-electron pairs in the converter, which are captured in the next accelerator section. By selecting the phase of the radiofrequency power to the subsequent accelerator sections (3) to be either the same as or opposite to that in the first section, either electrons or positrons are accelerated in the rest of the machine. The charged-particle beam is energy-analyzed, transported to the experimental room, and focused into a nearly parallel beam by the bending (5) and focusing (4) magnets. The analyzed beam then impinges on the thin Si single-crystal bremsstrahlung target (6), and the transmitted beam is swept out of the 0° line of sight with the sweeping magnet (7). The collimated beam of forward bremsstrahlung photons is detected with the NaI(Tl) photon spectrometer (8).

Fig. 22. Collimation system. The graphite collimator limits the charged-particle beam diameter at the position of the last quadrupole focusing magnet. The lead collimators limit the part of the silicon crystal viewed by the photon spectrometer as well as the angular divergence of the forward bremsstrahlung beam.

B. Experiment

The experimental procedures for the observation of coherent bremsstrahlung (36) were similar to those of the channeling work (Section II.). The apparatus is shown in Figure 21. Positron and electron beams of energy 28 MeV were obtained from the Livermore electron linear accelerator, energy analyzed with a bending-magnet-and-slit system to an energy spread of less than 1%, collimated in such a way that the beam was nearly parallel (see below) when it was allowed to strike a 5 μ m thick single crystal of silicon. The charged-particle beam, after having passed through the crystal, was bent down at a 45° angle by a sweeping magnet into a 3 m long dumphole underground, at the end of which it was monitored by a plastic scintillator detector. The forward beam of bremsstrahlung photons produced in the silicon crystal was itself collimated (see below) and viewed with a 12.5 cm dia. by 15 cm thick NaI(Tl) photon spectrometer positioned 5 m downstream from the silicon crystal. The 1.25 cm dia. silicon crystal was cut so that the short dimension (5 μ m) was nearly parallel to the $\langle 111 \rangle$ crystallographic direction, and was mounted on a goniometer capable of rotating the crystal through a two-dimensional angular range in 0.04 mrad steps.

The collimation system, which limits the momentum transferred by the incident charged particle to the crystal lattice, is shown in Figure 22. The maximum (full angle) beam divergence allowed was 4 mrad, corresponding to an optimum (full angle) divergence of half this value. However, careful tuning

of quadrupole magnets in the beam transport system resulted in a beam quality which was considerably better than these geometrical limits. This was borne out by the observation that positron-transmission measurements performed both with this set and with a much more restrictive set of collimators yielded essentially the same apparent channel widths. The upstream 1.6 cm dia. carbon collimator was selected to reduce the bremsstrahlung yield from that background source. Although the silicon crystal target was 1.25 cm in diameter, the downstream 0.5 cm diameter lead collimator and the 45 cm thick, 0.95 cm diameter lead collimator positioned directly in front of the NaI detector allowed it to view only the central area of the silicon target.

The orientation of the single crystal mounted in the goniometer was determined by the channeling response of transmitted positrons. The single crystal was initially grown and prepared with the $\langle 111 \rangle$ direction nearly normal to its surface. It was mounted on the inner gimbal ring of the goniometer and adjusted until the crystal showed no optical distortion. A positron mapping was performed to locate the string position and the (110) planes. This was accomplished by measuring the transmitted positron beam with a plastic scintillator as a function of the goniometer settings, as was discussed in Section II, and observing the large increase in the transmitted positron intensity when the crystal was swept through a channeling direction. This technique allowed the

crystal to be oriented to within 0.1 mrad, an uncertainty much smaller than the probably beam divergence involved.

The electronics and data-recording equipment were straightforward. The amplified output signals from the NaI spectrometer were split and fed both to a 1024-channel pulse-height analyzer having a threshold for valid events (well above noise level) corresponding to 162 KeV photons and to a single-channel analyzer having a threshold of 12.5 MeV for normalization purposes. Both analyzers were gated by a trigger pulse from the linear accelerator so that events occurring from cosmic rays and other machine-off background sources were reduced to a negligible rate. The counting rate of stored pulses was monitored and used to hold the beam intensity at a (low) constant level, so that pile-up corrections were small (<3%). A ^{22}Na γ -ray source was used to calibrate the energy scale. The accelerator was operated at 360 Hz (1 μs pulses); the experimental runs each were a few hours long, during which the counting rate never exceeded 10 sec^{-1} .

Eight kinds of data runs were taken, for both incident positrons and electrons and for each of four orientations of the target crystal: on-channel, on-shoulder, compound, and random. In the on-channel position, the particle beam was collinear with the $\langle 111 \rangle$ string direction (within the limits of divergence of the beam). The on-shoulder spectrum was measured with the particle beam incident along a (110) plane, 15 minutes of arc from the string direction. In the compound position, the particle beam was incident along a (110) plane,

50.5 minutes of arc from the string direction. Finally, the random-position spectra were measured at an orientation selected far from the string direction and major planes. The electron beam intensity was about three times as great as the positron beam intensity. Four electron spectra were measured with a high-energy-level (≥ 12.5 MeV) normalization of 15K counts and one compound spectrum was normalized to 30K counts. Four positron spectra were measured with a high-energy-level normalization of 5K counts and one compound spectrum was normalized to 10K counts.

C. Discussion of Data

The results are shown in Figures 23-26. Figure 23 shows the unnormalized photon spectra for the four positron runs, and Figure 24 shows those for the electron runs. The on-shoulder spectra (Figures 23b and 24b) and the on-channel spectrum for electrons (Figure 24a) show the enhancement of low-energy bremsstrahlung (relative to the random spectra shown in Figures 23d and 24d) expected from the results of the channeling experiment. Since the positrons, being positively charged, are repelled from the lattice sites (the atomic nuclei) when the beam is directed along the string direction, bremsstrahlung production in general is inhibited for this case, the coherence effect is suppressed, and hence the spectrum of Figure 23a does not show any significant low-energy enhancement. Indeed, the present collimation assured that the maximum beam divergence still lay within the channeling half angle

Fig. 23. Unnormalized photon spectra for incident positrons: (a) on-channel spectrum, (b) on-shoulder, (c) compound, (d) random.

Fig. 24. Unnormalized photon spectra for incident electrons: (a) on-channel spectrum, (b) on-shoulder, (c) compound, (d) random.

which was measured for this crystal in the channeling experiment. Therefore, one can assume that the positrons were well channeled and only dechanneled positrons contributed to the bremsstrahlung production, resulting in a photon spectrum comparable to the one for random orientation of the crystal.

The low-energy bremsstrahlung enhancement can be seen more clearly in Figure 25. Here are plotted the normalized differences between the spectra of Figures 23b and 23d (Figure 25a), Figures 24b and 24d (Figure 25b), and Figures 24a and 24d (Figure 25c). These normalizations equated the number of counts above 12.5 MeV for the various pairs of runs, on the reasonable assumption that all coherent effects in the high-energy regions of the bremsstrahlung spectra are negligible. The shoulder position was chosen to investigate the bremsstrahlung spectra for particles in the angular range where the "shoulders" of the channeling response are prominent. The low-energy bremsstrahlung enhancement for on-shoulder incident positrons (Figure 25a) exceeds that of the comparable electron data (Figure 25b). This could be explained by taking into account the second-Born-approximation for those two cases. The influence of axial channeling is dramatized by the large low-energy enhancement for on-channel electrons (Figure 25c); presumably this results from the electrons being attracted to the string of atomic nuclei, as contrasted with the case for positrons.

The photon spectra for the cases when the orientation of the silicon crystal, relative to the direction of the

Fig. 25. Normalized difference spectra, showing the low-energy bremsstrahlung enhancement: (a) on-shoulder-minus-random spectrum for positrons, (b) on-shoulder-minus-random spectrum for electrons, (c) on-channel-minus-random spectrum for electrons.

incident beam, was adjusted for compound interference are shown in Figures 23c and 24c. Both these spectra contain a striking peak near 500 KeV, although the peak is at least twice as prominent in the positron data (Figure 23c). The kinematics of coherent bremsstrahlung results in the prediction of a clustering of coherent bremsstrahlung strength near 0.5 MeV for the compound interference position chosen here for study, in agreement with these results. Although the charged-particle beam optics were not precisely the same for the two cases, it still is likely that channeling, with perhaps some contribution from the second-Born-approximation effect, account for the relatively greater enhancement of the coherent peak in the positron data. However, the quality of the data is insufficient to draw any conclusions regarding the expected fine structure (see Section A. above).

We also note that for the shoulder position a coherent bremsstrahlung peak should occur at 130 keV and higher order peaks approximately at integral multiples of this energy. However, the lowest-order shoulder peak is below the threshold set on the NaI detector and the higher order peaks are too weak to be discernable. Higher order peaks also should occur in the compound position spectra. Such peaks are predicted to lie near 1.1 MeV and 1.7 MeV, but should have intensities much smaller than the one near 0.5 MeV. Figure 26 shows the data up to 4 MeV for these spectra; it does not appear that these or any other higher-order peaks have been observed. Also,

Fig. 26. Unnormalized photon spectra up to 4 MeV for the compound interference case: (a) for incident positrons, (b) for incident electrons.

in both the shoulder and compound positions planar channeling might have some influence on the data but no apparent effect is discernable (the (110) planar-channeling angles are approximately 1/3 of the $\langle 111 \rangle$ axial-channeling value).

A scaling law appropriate for small angles of incidence would vary from

$$k \propto \gamma^2 \quad \text{at low } \gamma \ (\gamma < 100)$$

to

$$k \propto \gamma \quad \text{at high } \gamma \ (\sim \text{GeV})$$

At larger angles of incidence, the scaling law approaches

$$k \propto \gamma$$

For fine structure, the scaling law has the form

$$k \propto \gamma^{x>2}$$

which leads to the coalescing of the fine structure into a broad peak as the curvature of the momentum pancake is reduced (as the incident energy increases).

IV. CONCLUSIONS

The channeling of 16 to 28 MeV positrons in single crystals of silicon has been observed to follow the behavior predicted by the Lindhard theory quite well. Specifically, the energy dependence of the measured widths was in accordance with the theoretical prediction. The measured half angles for the positron axial channeling dips were about 20% to 30% lower than expected. The best agreement was for the scattered particle response; however at lower energies and thicker crystals, multiple scattering effects were evident. Additionally, planar channeling of positrons was observed and makes it possible to orient the crystal by mapping the major planes.

The electron channeling response has a central dip suggestive of spiral motion about the atomic rows due to conservation of both transverse and angular momenta. The energy dependence of the half-widths indicates that the response has the same $E^{-1/2}$ form as the Lindhard theory, which is consistent with the idea that a critical angle for electron channeling exists independent of the actual mode of the particle trajectory.

The forward bremsstrahlung intensity has been established as an observable of the channeling phenomenon. Enhancement of the low-energy portion of the bremsstrahlung was observed with both positron and electron beams incident along the crystal axes. It has now been shown clearly that the low-energy

component is due to coherent bremsstrahlung. The spectral shape of the low-energy component has been examined and a specific peak of coherent bremsstrahlung for a compound-interference direction has been observed. The position of this peak is consistent with first-order theory within the experimental accuracy of the measurement.

It is clear that certainly channeling and perhaps the validity of the first Born approximation must be considered when studying coherent bremsstrahlung generated by relativistic positrons and electrons in the MeV region. The data gathered from this experiment highlight the significance of the former and suggest the investigation of the latter with more high-resolution experimental measurements.

ACKNOWLEDGMENT

The author is greatly indebted to Dr. S. D. Bloom for his outstanding guidance and motivation, and to Dr. B. L. Berman for his exceptional insight and "trouble-shooting" ability. The author would also like to thank R. C. Der for help in taking the data; Dr. J. M. Khan, Dr. T. M. Kavanagh, and Prof. C. Kittel for valuable discussions; T. C. Madden and the Bell Telephone Laboratories for providing the silicon crystals; and E. Dante, H. Fong, and the other accelerator operators for their wizardry in producing parallel positron and electron beams.

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APPENDIX A

Silicon Lattice Structure

The tetrahedral bonding of silicon atoms leads to a diamond lattice structure for the crystalline form of silicon as depicted in Figure A1. Crystalline silicon has a lattice constant (a) of $5.43 \text{ \AA}$ and a nearest neighbor distance of $2.35 \text{ \AA}$. In normalized units these values are 1408 and 608 respectively ($\hbar/2\pi = c = m = 1$). The major intersecting planes in the $\langle 111 \rangle$ and $\langle 110 \rangle$ directions are shown in Figure A2 and Figure A3, respectively. For the continuum string potential employed in the Lindhard equation, the interatomic string distance d_s must be averaged along crystal directions where the atoms are not uniformly separated. As a result in the $\langle 110 \rangle$ direction $d_s = \frac{\sqrt{2}}{2} a = 3.84 \text{ \AA}$ corresponding to the actual separation, whereas in the $\langle 111 \rangle$ direction, $d_s = \frac{\sqrt{3}}{2} a = 4.69 \text{ \AA}$. These values correspond to 992 and 1216 in normalized units. The actual separation along the 111 direction alternates between $\frac{\sqrt{3}}{4} a$ and $\frac{3\sqrt{3}}{4} a$. Also since silicon has a diamond lattice structure the planar separation for (110) planes is given by $a/4$, and $a/12$ for (112) planes.

The reciprocal lattice of silicon is similar to two face centered cubic lattices displaced along the diagonal of $(1/4 \ 1/4 \ 1/4)$ as depicted in Figure A4. The structure factor for the reciprocal lattice points has the values 64, 32 or zero as shown by the (110) planar map along the $\langle 111 \rangle$ direction in Figure A5. A convenient reciprocal lattice dimension

is the distance between consecutive planes normal to a principle lattice direction. In Figure A5, the distance between consecutive (111) reciprocal lattice planes, $\bar{A}_{111}$ is given by

$$\bar{A}_{111} = \frac{1}{\sqrt{3}} \frac{2\pi}{a}$$

which for silicon = 2.58×10^{-3} in normalized units. These reciprocal lattice planes are indexed beginning at the origin with $l = 0, 1, 2$, etc. as depicted in Figure A5. Figure A6 is a map of the $l = 0$ (111) plane in the silicon reciprocal lattice.

Fig. A-1. Silicon crystal structure. Solid circles are either at corners or face-centered; open circles are on body diagonals.

Fig. A-2. Major intersecting planes in the $\langle 111 \rangle$ direction.

Fig. A-3. Major intersecting planes in the $\langle 110 \rangle$ direction. All listed planes are perpendicular to the face of the figure.

Fig. A-4. Reciprocal lattice of silicon. Solid circles represent lattice points with structure factor of 64; crosses, structure factor of 32.

Fig. A-5. Map of reciprocal lattice (110) plane. The (110) plane is defined by the $\langle 111 \rangle$ and $\langle 112 \rangle$ directions in the reciprocal lattice.

Fig. A-6. Map of reciprocal lattice (111) plane. The $l = 0$ (111) plane of the reciprocal lattice contains the origin and is normal to the $\langle 111 \rangle$ direction and the (112) and (110) planes.

APPENDIX B

Coherent Bremsstrahlung Computer Program

In the phenomenon known as coherent bremsstrahlung, the interaction involves discrete values of allowed lattice recoil momenta which are restricted to reciprocal lattice vectors according to the Bragg condition for coherent reflection. Indeed, the reciprocal lattice itself represents the classical array in momentum space of allowed lattice recoil momenta for any coherent interaction whatsoever. The interference effects associated with coherently produced bremsstrahlung can be explained by examining the momentum vector diagram with the reciprocal lattice as a basis. The reciprocal lattice of silicon is discussed in Appendix A.

Consider an incident particle with momentum $\bar{P}_1$. We want to determine all possible momentum vector combinations which lead to the generation of a photon with momentum $\bar{k}$ collinear with $\bar{P}_1$. From energy conservation, we know that for relativistic particles

$$\gamma_1 mc^2 = \gamma_2 mc^2 + (h/2\pi)kc + \frac{q^2}{2M} \quad , \text{ or} \quad (B1)$$

in normalized units, neglecting the last term

$$\gamma_1 = \gamma_2 + k \quad (B2)$$

For momentum conservation we have

$$\gamma_1(1-1/2\gamma_1^2) = q \cos\beta + \gamma_2(1-1/2\gamma_2^2)\cos\alpha + k \quad (B3)$$

where $q \equiv$ lattice recoil momentum,

$\beta \equiv$ angle between q and γ_1 ,

$\alpha \equiv$ angle between γ_1 and γ_2 ,

and

$$q \sin\beta = \gamma_2(1-1/2\gamma_2^2)\sin\alpha \quad . \quad (B4)$$

We define

$$q_1 \equiv q \cos\beta \quad , \quad (B5a)$$

$$q_2 \equiv q \sin\beta \quad , \quad (B5b)$$

and

$$\begin{aligned} Q &\equiv \left\{ \left\{ \gamma_2(1-1/2\gamma_2^2) \right\}^2 - q_2^2 \right\}^{1/2} \\ &= \gamma_2(1-1/2\gamma_2^2)\cos\alpha \quad , \end{aligned} \quad (B5c)$$

then we make the following approximation,

$$Q = \gamma_2(1-1/2\gamma_2^2) \left(1 - q_2^2 / \left\{ \gamma_2^2(1-1/2\gamma_2^2)^2 \right\} \right)^{1/2} \quad (B6a)$$

$$Q \approx \gamma_2(1-1/2\gamma_2^2) \left(1 - q_2^2 / \{ 2\gamma_2^2(1-1/2\gamma_2^2)^2 \} \right) \quad (B6b)$$

$$Q \approx \gamma_2(1-1/2\gamma_2^2) \{ 1 - q_2^2 / 2\gamma_2^2 \} \quad . \quad (B6c)$$

We can then express momentum conservation as follows,

$$\gamma_1(1-1/2\gamma_1^2) - \gamma_2(1-1/2\gamma_2^2)(1-q_2^2/2\gamma_2^2) - k = q_1 \quad . \quad (B7)$$

Rearranging and simplifying yields,

$$\gamma_2 = \frac{1 + q_2^2}{1/\gamma_1 + 2q_1} \quad . \quad (B8)$$

Then using energy conservation we get,

$$k = \frac{\gamma_1(2\gamma_1 q_1 - q_2^2)}{1 + 2\gamma_1 q_1} \quad (B9a)$$

or

$$\frac{k}{\gamma_1} = X = \frac{2\gamma_1 q_1 - q_2^2}{1 + 2\gamma_1 q_1} \quad (B9b)$$

This equation represents the lower boundry of the momentum pancake and thereby determines the maximum value for k of coherent bremsstrahlung generated with q_1 and q_2 at γ_1 incident energy. The minimum value for k generated by any fixed q and γ_1 will be set by the collimation of the photon beam. This results physically from restricting the emission angle θ_k in the experiment. Thus, the coherent peak will have a bandwidth given by (35),

$$X_{\text{coll}} = \frac{X_{\text{peak}}}{1 + \phi_c^2 (1 - X_{\text{peak}})} \quad (B10)$$

where

$$X_{\text{peak}} = \frac{2\gamma_1 q_1 - q_2^2}{1 + 2\gamma_1 q_1} \quad (B11)$$

and ϕ_c is the collimation angle expressed in units of γ_1^{-1} .

Collimation also reduces the intensity of the incoherent background, since the angular distribution is of the form

$$d\sigma(\theta_k) = C \frac{\phi_k d\phi_k}{(1 + \phi_k^2)^2} ; \quad \phi_k \equiv \gamma \theta_k \quad (B12)$$

and collimation to an angle θ_c gives a reduction by the factor

$$f = \frac{\int_0^{\theta_c} d\sigma}{\int_0^{\infty} d\sigma} = \frac{\phi_c^2}{1 + \phi_c^2} \quad (B13)$$

The integration of the coherent differential cross-section has been treated extensively (17, 35, 37). The result for the intensity spectrum, with both coherent and incoherent contributions, takes the form

$$\frac{k}{\sigma_0} \frac{d\sigma}{dk} = \{1 + (1-X)^2\} \{\psi_1^C + \psi_1^I\} - \frac{2}{3}(1-X) \{\psi_2^C + \psi_2^I\} \quad (B14a)$$

where

$$\psi_1^C = \frac{(2\pi)^2}{2a^3} \sum_g |S(g)|^2 e^{-Ag^2} F(g^2) \cdot \frac{\delta(g_2^2 + g_3^2)}{\{g_1 + \theta(g_2 \cos \alpha + g_3 \sin \alpha)\}^2} \quad (B14b)$$

$$\psi_2^C = 3 \frac{(2\pi)^2}{a^3} \sum_g |S(g)|^2 e^{-Ag^2} F(g^2) \cdot \frac{\delta^2(g_2^2 + g_3^2) \{g_1 + \theta(g_2 \cos \alpha + g_3 \sin \alpha) - \delta\}}{\{g_1 + \theta(g_2 \cos \alpha + g_3 \sin \alpha)\}^4} \quad (B14c)$$

$$\psi_1^I = 4 + 4 \int_{\delta}^1 (1 - e^{-Ag^2}) F(g^2) (g - \delta)^2 g dg \quad (B14d)$$

$$\psi_2^I = \frac{10}{3} + 4 \int_{\delta}^1 (1 - e^{-Ag^2}) F(g^2) \cdot \{g^2 - 6\delta \ln(g/\delta) + 3\delta^2 - \frac{4\delta^3}{g}\} g dg \quad (B14e)$$

where the sum is over all values of reciprocal lattice vectors g with

$$g_1 + \theta(g_2 \cos \alpha + g_3 \sin \alpha) > \delta \quad (B15a)$$

$$\delta = \frac{1}{2\gamma_1} \frac{x_{\text{peak}}}{1 - x_{\text{peak}}} \quad (B15b)$$

We note that

$$\delta \equiv \text{the minimum recoil,} \quad (\text{B16a})$$

$$S(g) \equiv \text{the crystal structure factor,} \quad (\text{B16b})$$

$$e^{-Ag^2} \equiv \text{the Debye-Waller factor,} \quad (\text{B16c})$$

$$F(g^2) \equiv \text{the atomic form factor,} \quad (\text{B16d})$$

$$\theta \equiv \text{the polar angle with respect to } g_1, \quad (\text{B16e})$$

$$\alpha \equiv \text{the azimuthal angle with respect to } g_1. \quad (\text{B16f})$$

Also we note

$$\frac{k}{\sigma} \frac{d\sigma}{dk} \equiv I = I^c + I^i \quad (\text{B17})$$

where "c" and "i" refer to the coherent and incoherent contributions to Equation B17. The incoherent contribution can be determined by numerical integration of ψ_1^i and ψ_2^i which depend weakly on δ and as a good approximation can be evaluated at $\delta = 0$ (35).

The form of the coherent contribution can be simplified by the approximation that $g_1 = 0$. This limits the treatment to the first plane of the reciprocal lattice. Now we note, for

$$\tau \equiv \theta/\delta \quad ; \quad \theta \ll 1 \quad (\text{B18a})$$

with the condition,

$$g_2 \cos \alpha + g_3 \sin \alpha > \tau^{-1} \quad (\text{B18b})$$

we obtain

$$\begin{aligned} \psi_1^c(\delta) = & \frac{(2\pi)^2}{\delta \cdot 2\tau^2 a^3} \int_g |S(g)|^2 e^{-Ag^2} F(g^2) \cdot \\ & \cdot \frac{g^2}{(g_2 \cos \alpha + g_3 \sin \alpha)^2} \end{aligned} \quad (\text{B19a})$$

$$\psi_2^C(\delta) = \frac{3(2\pi)^2}{\delta^4 \tau^3 a^3} \sum_g |S(g)|^2 e^{-Ag^2} F(g^2) \cdot \frac{g^2 (g_2 \cos \alpha + g_3 \sin \alpha - \tau^{-1})}{(g_2 \cos \alpha + g_3 \sin \alpha)^4} \quad (B19b)$$

We next investigate the formulation under the condition of equality for Equation B18b,

$$g_2 \cos \alpha + g_3 \sin \alpha = \tau^{-1} \quad (B20a)$$

which occurs at a peak discontinuity in the spectrum given by

$$X_{\text{peak}} = \frac{2\theta \gamma_1 \tau^{-1}}{1 + 2\theta \gamma_1 \tau^{-1}} \quad (B20b)$$

indicating that X_{peak} is a function of θ and τ . At the discontinuity, ψ_2^C vanishes and we have

$$I^C(X_{\text{peak}}) = \gamma_1 \Omega(X_{\text{peak}}) \frac{(2\pi)^2}{a^3} |S(g)|^2 e^{-Ag^2} F(g^2) g^2 \quad (B21a)$$

where

$$\Omega(X_{\text{peak}}) = \{1 + (1 - X_{\text{peak}})^2\} (1 - X_{\text{peak}}) / X_{\text{peak}} \quad (B21b)$$

Since τ is determined by α , $I^C(X_{\text{peak}})$ varies with θ and α for fixed γ_1 and the optimum intensity is dependent upon the reciprocal lattice structure. $I^C(X_{\text{peak}})$ measures the relative contribution of points along the rows orthogonal to α in the first plane of the reciprocal lattice structure. θ will determine the total intensity since it sets δ once τ is fixed by α . An equivalent development which includes polarization is given elsewhere (17,35).

The foregoing theory is based upon the first Born approx-

imation and is considered valid for high energies, i.e.

$\gamma_1 \gg 1$ and $\gamma_2, k \gg 1$. The present development restricts itself to the first plane of the reciprocal lattice and does not properly treat photons with energies of the order of $k = 1$ where significant contributions to coherent bremsstrahlung are observed at low relativistic energies. These limitations deal with the absolute intensity of the coherent bremsstrahlung and do not impair one's ability to calculate the qualitative features of the spectra, namely the position and structure of the peaks resulting from the kinematics.

Calculations based on the present theory are adequate to investigate the qualitative shape of coherent bremsstrahlung spectra. A program written by Schwitters (27) for evaluating experiments in the GeV range at SLAC and CEA has been modified for use at lower relativistic energies. The essential modification was to introduce the curvature term in the kinematics and allow an independent calculation of the multiple scattering angle since that parameter increases with decreasing energy. Both first (beam) and second (photon) collimation has been included with revised algorithms to account for the inability of a discrete computer calculation to represent a finite band smaller than the energy increments used in the program. Multiple scattering is treated by "rocking" the crystal about the incident particle direction and weighting the results of separate calculations at different mesh points by a normal distribution function related to the mean multiple

scattering angle. The size of the multiple scattering mesh can be varied to trade-off computer running time for accuracy of the simulation. The program contains fundamental constants and data which enable the user to compute coherent bremsstrahlung from diamond, beryllium, or silicon single crystals.

Four input data cards are used to run the program:

Card 1 Format (18A4)

 Name Self Explanatory

Card 2 Format (11, F9.4, 5F10.4)

NCRSTL 1 - Diamond

 2 - Beryllium

 3 - Silicon

EGEV Energy in GeV

UP SLAC Code (Set at 0)

THICK Crystal Thickness (mils)

ANG SLAC Code (Set at -1)

U Second collimation angle in units
 of γ^{-1}

SI Mean multiple scattering angle in
 units of γ^{-1}

Card 3 Format (3F10.4)

A Euler angles of target in crystal
 holder (degrees)

B Same as above

C Same as above

NPL Major face of the crystal

Card 4 Format (4F10.4)

THV	Vertical angle of incidence for beam striking target in crystal holder (mrad)
THH	Horizontal angle of incidence for beam striking target in crystal holder (mrad)
THVO	Set to zero
THHO	Set to zero

Additionally, by changing program cards, the following options are available:

For a 3 x 3 multiple scattering mesh

DATA NHINT/3/,XHSD/1./

DATA NVINT/3/,XVSD/1./

For a 9 x 9 multiple scattering mesh

DATA NHINT/21/,XHSD/2./

DATA NVINT/21/,XVSD/2./

For no multiple scattering

DATA NHINT/2/,XHSD/0/

DATA NVINT/2/,XVSD/0/

The size of the reciprocal lattice scan can be changed by setting NSCAN to the desired value (the maximum Miller index of interest).

A listing of the program is available in the library-storage system of Lawrence Livermore Laboratory under the name MULTSC.

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Printed in the United States of America
Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy \$ ____*; Microfiche \$2.25

* Pages

~~1-50
51-150
151-325
326-500
501-1000~~

NTIS
Selling Price

~~\$4.00
\$5.45
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\$10.60
\$13.60~~

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