Planar channeling radiation by relativistic electrons in different structures of silicon carbide

B Azadegan¹, S B Dabagov²,³ and W Wagner⁴

¹ Sabzevar Tarbiat Moallem University - P.O. 297, Sabzevar, Iran
² INFN, Laboratori Nazionali di Frascati - Via E. Fermi 40, 00044 Frascati (RM), Italy
³ RAS - P.N. Lebedev Physical Institute - Leninsky Pr. 53, 119991 Moscow, Russia
⁴ Helmholtz-Zentrum Dresden-Rossendorf - P.O.Box 510119, 01314 Dresden, Germany

E-mail: azadeganb@gmail.com

Abstract. Spectral distributions of channeling radiation by relativistic electrons channeled in different crystallographic planes of different types of polytype silicon carbide crystals such as hexagonal, zincblende and rhombohedral are presented. For every structure we have found the planes where the emission of channeling radiation is possible. Using the Doyle-Turner approximation to the atomic scattering factor and taking into account thermal vibrations of crystal atoms, the continuum potentials for different planes in different structures of a SiC single crystal have been calculated. In the framework of quantum mechanics, the theory of channeling radiation was applied to calculate transverse electron states, transition energies, radiation linewidths, the depth dependence of the occupation of quantum states and spectral-angular distributions of channeling radiation. At electron energies larger than 100 MeV, the trajectories, velocities and accelerations of channeled electrons have been obtained by means of classical mechanics, and the spectral-angular distributions were calculated by means of classical electrodynamics using realistic trajectories, velocities and accelerations of channeled electrons. Specific properties of planar channeling radiation generated in different structures of SiC are discussed.

1. Introduction

Channeling radiation (CR) is emitted by relativistic charged particles during passing through a single crystal nearly parallel to some crystallographic axis or plane. Electron CR has mainly been studied on monatomic crystals such as diamond [1, 2, 3], Si [4, 5, 6], Ge [7, 8] and on metals (e.g. Be, Ni, Sb, W [9, 10, 11]). Binary or polyatomic crystals (e.g. LiH [12], LiF [13, 14], GaAs, ruby [15]) have scarcely been utilized. Most of the above mentioned crystals are characterized by a cubic lattice. In such crystals, intense CR is observed from channeling along planes with small indices such as (100), (110) and (111). In our previous papers [16, 17] we investigated CR generated in different planes of a quartz crystal (SiO₂) which has a hexagonal structure. The more complicate structure of the binary quartz crystal (compared with cubic crystals such as, e.g., diamond, Si or Ge) allows for planes with relatively large indices, which have rather deep continuum potentials favouring CR emission. One may observe some specific properties of CR also on other types of crystals. The most remarkable feature of the silicon carbide (SiC) crystal structure is its polytypism. There is a great variety of SiC polytypes. Therefore, it has become accepted practice to refer to the cubic polytype as b-SiC and to all non-cubic structures (hexagonal and rhombohedral) as a-SiC. Despite the large number of well documented SiC
polytypes, only very few of them are considered to be thermodynamically stable. However, there appear to be five small-period polytypes (2H, 3C, 4H, 15R and 6H) which are considered as the basic SiC structures because they are found to occur most frequently. In the present paper, planar CR on 3C-SiC (zincblende), 4H-SiC (hexagonal) and 9R-SiC (rhombohedral) is investigated.

2. Theory

2.1. Planar channeling radiation

For planar channeling, the relativistic particle must enter the crystal under a small incidence angle with respect to the crystal plane considered. The description of channeling is based on the division of the particle motion into a longitudinal and a transverse component. Since in first approximation the longitudinal component along the channeling plane is not affected by forces, the velocity in this $z$-direction is actually nearly constant, $v_z \approx c$. However, under channeling condition, the transverse momentum of the channeled particle, $p_x$, is small compared to the longitudinal one, $p_z$. Therefore, its transverse energy may be defined by the expression

$$E_x = \frac{p_x^2}{2m\gamma} + V(x)$$

where $m\gamma$ is the relativistic mass and $\gamma$ is the Lorentz factor [18]. In order to describe the radiation emitted by the charged particle during channeling, the applicability of both the classical and the quantum theory has to be considered.

2.2. Continuum potential

Since the longitudinal component of the electron velocity approaches the speed of light, $c$, the crystal plane is assumed to be charged continuously, and $V(x)$ is approximated by the continuum potential [19]. This potential has the periodicity of the lattice. Therefore, its expansion into a Fourier series represents its most general form which reads

$$V(x) = \sum_{n=1,2,...} V_n \exp(ingx) \quad n = ... -1, 0, 1, 2, ...$$

where $V_n$ denote the Fourier coefficients of the periodic potential. Using the Doyle-Turner approach [21] for the electron-atom interaction, they can be written as

$$V_n = -\frac{2\pi a_0 e^2}{V_c} \sum_j \exp[-M_j(\vec{g})] \exp(-i\vec{g} \cdot \vec{r}_j) \sum_{i=1}^4 a_i \exp[-\frac{1}{4} \frac{b_i}{4\pi^2} (ng)^2]$$

where $V_c$ is the volume of unit cell, $a_0$ is the Bohr radius, $e$ is the electron charge, $\vec{r}_j$ represents the coordinates of the $j$ atoms in the unit cell, $a_i$ and $b_i$ are tabulated coefficients [21], and $M_j(\vec{g}) = g^2 \langle u_j^2 \rangle / 2$ denotes the Debye-Waller factor which describes the thermal vibration of the $j^{th}$ atom by a mean-squared amplitude $\langle u_j^2 \rangle$. The term $\sum \exp(-i\vec{g} \cdot \vec{r}_j)$ in (3) is the structure factor of the crystal. The structure factor determines those sets of Miller indices, $(hkl)$, for which the reflections from the corresponding planes are strong.

2.3. Classical description of planar channeling radiation

In the framework of the classical model, the scattering from the ordered crystal atoms becomes coherent now, causing an oscillatory motion of the electrons along the corresponding plane of atoms. Considering this oscillatory motion as an accelerated one within the rest frame of the electron, it emits electromagnetic radiation called channeling radiation. Although the oscillation
frequency, $\omega_0$, is rather low and corresponds to a radiation energy, $\hbar \omega_0$, in the optical region, relativistic effects such as the Lorentz contraction of the longitudinal coordinate and the Doppler effect transform the energy of emitted CR photons observed in beam direction into the domain of X-rays.

The equation of motion for the relativistic particle in the one-dimensional continuum potential, $V(x)$, has the form

$$\gamma m \ddot{x} = -\frac{\partial V(x)}{\partial x}. \quad (4)$$

The initial conditions are: the point of incidence into the crystal, $x(0) = x_0$, and the transverse momentum $p_x(0) = p \theta_0$ ($\theta_0$ is the angle of incidence with respect to the plane) which define the initial transverse energy (1) as

$$E_x = \frac{p^2 \theta_0^2}{2 \gamma m} + V(x_0). \quad (5)$$

The energy density radiated into a solid angle $d\Omega$ and a frequency interval $(\omega, \omega + d\omega)$ has the following form [18]

$$\frac{d^2 E}{d\omega d\Omega} = \frac{e^2}{4\pi^2 c} \left| \int_0^\tau \exp[i(\omega t - \vec{k} \cdot \vec{r})] \frac{\vec{n} \times ((\vec{n} - \vec{\beta}) \times \vec{\beta})}{(1 - \vec{\beta} \cdot \vec{n})^2} dt \right|^2 \quad (6)$$

where $\vec{\beta} = \vec{\gamma}(t)/c$ is the particle velocity, $\vec{r}(t) = \vec{v} t + x(t)$ is its trajectory, $\vec{k} = \omega \vec{n}/c$ is the wave vector, $\vec{n}$ is the unit vector defining the direction of photon emission, and $\tau$ is the time-of-flight of the particle through the crystal. Classical calculations of CR spectra are based on (6).

2.4. Quantum description of planar channeling radiation

In the framework of quantum mechanics, the transverse motion of planar channeled electrons of mass $\gamma m$ may be described by a one-dimensional Schrödinger equation which contains the averaged potential of the crystal. This motion is restricted to discrete (bound) channeling states of the planar continuum potential. Spontaneous transitions between these eigenstates lead to the emission of CR, the energy spectrum of which is consequently characterized by a line structure of possible photon energies. For electrons of relatively low energy, the quantum theory of CR is based on a Bloch-wave solution

$$\psi(x) = \exp(i k x) \sum_n c_n \exp(i n g x) \quad n = ... -1, 0, 1, 2, ... \quad (7)$$

of the Schrödinger equation

$$-\frac{\hbar^2}{2\gamma m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x) \quad (8)$$

for incident particles passing through the periodic planar potential $V(x)$. Here $\vec{k}$ is the electron wave vector, and $\vec{g}$ is the reciprocal lattice vector of the plane. Substitution of (2) and (7) into (8) reduces the problem to the calculation of the eigenvalues of a matrix $A$, which in the planar case consist of the components

$$A_{nm} = V_{n-m} \text{ for } (n \neq m); \quad A_{nn} = \frac{\hbar^2}{2\gamma m} (k + ng)^2 + V_0. \quad (9)$$

Since the potential as well as the eigenvalues converge very fast, one can restrict the solution to 21 Bloch functions what leads to a $21 \times 21$ matrix problem.
For planar CR directed along the electron motion, the spontaneous transition rate per unit of solid angle, per unit of photon energy, per unit of crystal thickness and per electron is given by

\[
\frac{d^3N_{\text{CR}}(i \rightarrow f)}{d\Omega dE d\gamma dz} = \frac{\alpha \lambda_k^2}{\pi c \hbar} \int dk E_k^0 \left| \frac{d}{d\gamma} \langle \psi_{kf} \mid \psi_{ki} \rangle \right|^2 \frac{\left( \Gamma_k/2 \right)}{(E_\gamma - E_k^{(0)})^2 + 0.25 \Gamma_k^2} P_{ki}(z) \tag{10}
\]

where \( \langle \psi_{kf} \mid \frac{d}{d\gamma} \mid \psi_{ki} \rangle \) is the transition matrix element, \( P_{ki}(z) \) gives the occupation probability of the channeling state \( i \) as function of initial population and crystal thickness, \( E_k^0 = 2\gamma^2(\epsilon_{ki} - \epsilon_{kf}) \) means the photon energy of the transition \( i \rightarrow f \), and \( \Gamma_k \) is the intrinsic CR linewidth. It should be underlined that the integral in (10) has to be taken over the Bloch momenta, \( k \). A second integral may be taken over the occupation \( P_i \) of the state \( i \) along a given crystal thickness \( z = L \) to calculate the spectral-angular distribution of CR. Both the intrinsic CR linewidth and the occupation probability of the state \( i \) are calculated as given in [3] and [17], respectively.

2.5. Classical versus quantum model for planar CR on SiC

The applicability of classical or quantum approach for CR calculations may be checked by estimation of the number of states within the continuum potential [18]. At low energies (units up to tens of MeV) the particle motion has quantum character. The line structure of the CR spectrum is clearly pronounced, while band-structure effects appear for high lying levels. Calculations and measurements for main crystallographic directions of Si and diamond crystals show that the number of bound states is relatively small for electron energies less than 100 MeV. Therefore, a quantum mechanical description of CR is necessary. With increasing electron energy, the density of bound states increases what eventually leads to an overlap of states while band-structure effects become less important. This situation can be handled by a classical calculation [20].

![Figure 1](image1.png)  
**Figure 1.** Continuum potential of the (1120) plane of a 4H-SiC crystal and bound states for electrons of energy 20 MeV.

![Figure 2](image2.png)  
**Figure 2.** Continuum potential of the (1120) plane of a 4H-SiC crystal and bound states of channeled electrons of energy 200 MeV.

3. Crystals

Polytypes of SiC differ in the ordered sequence of closely packed Si-C biplanes along the stacking axis (c-axis). Each polytype has a symbol consisting of a number followed by a letter, where the number denotes the number of layers in one repeat unit along the c-axis and the letter denotes the symmetry. There is one cubic (C) polytype: 3C-SiC. Other polytypes have either hexagonal (H) or rhombohedral (R) symmetry. The primitive unit cell of 3C-SiC contains one Si-C unit, whereas the primitive unit cells of the nH or 3nR polytypes contain n Si-C units.
The coordinates of the Si and C atoms in the hexagonal coordinates system are
\[
\begin{align*}
\vec{a}_1 &= a_0 \hat{x} - \sqrt{3} a_0 \hat{y}, \\
\vec{a}_2 &= a_0 \hat{x} + \sqrt{3} a_0 \hat{y}, \\
\vec{a}_3 &= c \hat{z}
\end{align*}
\]
with \(a_0 = 3.0805 \textrm{Å} \) and \(c = 10.0848 \textrm{Å} \) [22].

The coordinates of the Si and C atoms in the hexagonal coordinates system are
\[
\begin{align*}
\text{Si(I)} : & \{0, 0, Z_1 \}, \{0, 0, (Z_1 + 1/2)c \} \\
\text{C(I)} : & \{0, 0, Z_2 \}, \{0, 0, (Z_2 + 1/2)c \} \\
\text{Si(II)} : & \{\frac{1}{2} a, \frac{1}{2} a, Z_3 \}, \{\frac{1}{2} a, \frac{1}{2} a, (Z_3 + 1/2)c \} \\
\text{C(II)} : & \{\frac{1}{2} a, \frac{1}{2} a, Z_4 \}, \{\frac{1}{2} a, \frac{1}{2} a, (Z_4 + 1/2)c \}
\end{align*}
\]
with \(Z_1 = 0.0, Z_2 = 0.1875, Z_3 = 0.249825 \) and \(Z_4 = 0.437325 \). In this form, a crystal plane is given by a set of four indices \((hkl)\) with \(i = -(h + k)\) and \(h, k, l\) being Miller indices.

### 3.2. SiC(3C)

The second unit-cell SiC polytype is cubic (space group \(\text{Td}^{2}_{4} \text{F} 43\text{m}, \) unit cell length \(a = 4.36 \textrm{Å}\)).

The primitive vectors in the Cartesian coordinates system are
\[
\vec{a}_1 = \frac{1}{2} a (\hat{y} + \hat{z}), \quad \vec{a}_2 = \frac{1}{2} a (\hat{z} + \hat{y}), \quad \vec{a}_3 = 1 a (\hat{x} + \hat{y})
\]

The coordinates of Si and C atoms in the hexagonal coordinates system are
\[
\begin{align*}
\text{Si} : & \{0, 0, 0\}, \quad \text{C} : \{\frac{1}{2} a, \frac{1}{2} a, \frac{1}{2} a\}
\end{align*}
\]
For cubic crystals, the three Miller indices \(h, k, l\) describe crystallographic axes and planes.

### 3.3. SiC(9R)

The third unit-cell SiC polytype is rhombohedral (space group \(\text{C}_{3v}^{2} \text{R} 3\text{m}, a = 3.018 \textrm{Å}, c = 22.177 \textrm{Å}\)). The primitive vectors in the Cartesian coordinates system are
\[ \mathbf{a}_1 = \frac{1}{2} \mathbf{a} \hat{x} + \frac{1}{2\sqrt{3}} \mathbf{a} \hat{y} + \frac{1}{3} \mathbf{a} \hat{z}, \quad \mathbf{a}_2 = -\frac{1}{2} \mathbf{a} \hat{x} + \frac{1}{2\sqrt{3}} \mathbf{a} \hat{y} + \frac{1}{3} \mathbf{a} \hat{z}, \quad \mathbf{a}_3 = -\frac{1}{\sqrt{3}} \mathbf{a} \hat{y} + \frac{1}{3} \mathbf{a} \hat{z} \]

The coordinates of Si and C atoms are

\[ C(I) : \{0, 0, x_1c\}, \{0, 0, x_2c\}, \{0, 0, x_3c\} \]

\[ Si(I) : \{0, 0, x_4c\}, \{0, 0, x_5c\}, \{0, 0, x_6c\} \]

with \( x_1 = 0.222, x_2 = 0.0, x_3 = -0.222, x_4 = 0.3055, x_5 = 0.0833, x_6 = -0.1388 \).

### 4. Calculations

#### 4.1. SiC(4H)

The calculated planar potential for electrons channeled along the (11\bar{2}0) plane of a 4H-SiC crystal, eigenvalues and Bloch bands for the two electron energies of 20 MeV and 200 MeV are shown in figures 1 and 2, respectively. When at 20 MeV the particle motion has clearly quantum character, because there are only four bound states and, hence, three separate CR lines in the spectrum (figure 3), at 200 MeV one observes 10 bound states. It seems that channeling at this energy has already classical character.

Our calculations of the depth dependence \( P_{kn}(z) \) of the occupation of bound and quasi-free states, performed for the electron energy of 20 MeV, showed that the statistical equilibrium of occupation of states is reached at a depth of only about 2\( \mu \)m. The total CR photon yield one obtains by integration of the occupation function over the entire crystal thickness. The result for a 5\( \mu \)m thick 4H-SiC crystal is presented in figure 3.

In order to classically calculate the spectral-angular distribution of CR for electrons of energy 200 MeV, one has to substitute into (6) the trajectories, velocities and accelerations of channeled electrons obtained from numerical solutions of the equation of motion (4) with the potential of the (11\bar{2}0) plane of the 4H-SiC crystal. Since different initial conditions lead to different trajectories and partial spectral-angular distributions of CR as well, one has to average over all possible trajectories. The result for a 5\( \mu \)m thick 4H-SiC crystal is given in figure 4.
4.2. SiC(3C)

The continuum potential calculated for the (110) plane of the cubic 3C-SiC crystal is shown in figure 5. The eigenvalues and Bloch bands correspond to an electron energy of 30 MeV. The potential is formed by a combination of Si and C atomic potentials. It shows alternating segregate potential wells, where the deep ones are formed by Si atoms and smaller modulations are caused by the C atoms. The CR spectrum simulated by means of (10) for electrons of energy 30 MeV channeled in the (110) plane of a 5µm thick 3C-SiC crystal is shown in figure 6.

4.3. SiC(9R)

The continuum potential of the (110) plane of a 9R-SiC crystal and the corresponding CR spectrum calculated for electrons of energy 30 MeV and a 5µm thick 9R-SiC crystal are presented in figure 7 and 8, respectively.

5. Summary

In the present paper, the quantum mechanical and the classical approach for the description of channeling radiation are explained and applied for simulations of planar electron channeling in different structures of the polytype SiC crystal. At electron energies less than 100 MeV, transverse transition energies, linewidths and spectra of channeling radiation have been calculated numerically applying the well-known many-beam formalism with thermally averaged Doyle-Turner potentials. For higher electron energies, the spectral-angular distributions of channeling radiation were calculated by means of the classical method. Realistic trajectories, velocities and accelerations of channeled electrons have been obtained, and they were used to calculate the photon spectra of channeling radiation according to classical electrodynamics.
References

[1] Gouanere M, Sillou D, Spighel M, Cue N, Gaillard M J, Kirsch R G, Poizat J-C, Remillieux J, Berman B L, Catillon P, Roussel I and Temmer G M 1982 Nucl. Instrum. Meth. 194 225

[2] Reiz I 1999 Diploma thesis (Darmstadt: Technical University); Genz H 2001 Proc. NATO Advanced Research Workshop on Electron-Photon Interaction in Dense Media (Nor-Hamberd, NAS Armenia)

[3] Azadegan B, Wagner W and Pawelke J 2006 Phys. Rev. B 74 045209

[4] Gouanere M, Sillou D, Spighel M, Cue N, Gaillard M J, Kirsch R G, Poizat J-C, Remillieux J, Berman B L, Catillon P, Roussel I and Temmer G M 1988 Phys. Rev. B 38 4352

[5] Andersen J U and Lægsgaard E 1980 Phys. Rev. Lett. 44 1079

[6] Kephart J O, Berman B L, Pantell R H, Datz S, Klein R R and Park H 1991 Phys. Rev. B 44 1992

[7] Park H, Svent R L, Kephart J O, Pantell R H, Berman B L, Datz S and Fearick R W 1983 Phys. Lett. 96A 45

[8] Chouffani K, Überall H, Genz H, Hoffmann-Staschek P, Nething U and Richter A 1999 Nucl. Instrum. Meth. B 152 479

[9] Andersen J U, Bonderup E, Lægsgaard E and Sørensen A H 1983 Phys. Scr. 28 308

[10] Gary C K, Fisher A S, Pantell R H, Harris J and Piestrup M A 1990 Phys. Rev. B 42 7

[11] Buschhorn G, Dietrich E, Kufner W, Rzepka M, Genz H, Grf H-D, Hoffmann-Staschek P, Nething U and Richter A 1997 Phys. Rev. B 55 6196

[12] Gary C K, Pantell R H, Özcan M, Piestrup M A and Boyers D G 1991 J. Appl. Phys. 70 2995

[13] Berman B L, Datz S, Fearick R W, Kephart J O, Pantell R H, Park H and Svent R L 1982 Phys. Rev. Lett. 49 474

[14] Svent R L, Pantell R H, Park H, Kephart J O, Klein R K, Datz S, Fearick R W and Berman B L 1984 Phys. Rev. B 29 52

[15] Freudewberger J, Genz H, Groening L, Hoffmann-Staschek P, Knupfer W, Morokhovskii V L, Morokhovskii V V, Nething U, Richter A and Sellschop J P F 1996 Nucl. Instrum. Meth. B 119 123

[16] Wagner W, Azadegan B, Grigoryan L Sh and Pawelke J 2007 EPL 78 56004

[17] Azadegan B, Grigoryan L Sh, Pawelke J and Wagner W 2008 J. Phys. B 41 325101

[18] Kumakhov M A and Weddel R 1991 Radiation of Relativistic Light Particles during Interaction with Single Crystals (Heidelberg: Spektrum)

[19] Lindhard J 1965 Kg. Danske Ved. Selsk. Mat. Fys. Medd. 14 34

[20] Bogdanov O V, Korotchenko K B and Pivovarov Yu L 2008 J. Phys. B 41 055004

[21] Doyle P A and Turner P S 1968 Acta Crystallogr. A 24 390

[22] Bernstein N, Gotsis H J, Papaconstantopoulos D A and Mehl M J 2005 Phys. Rev. B 71 075203