Polarization of radiation from axially channeled electrons

R. Fusina
Complex Systems Theory Branch, Code 4690, Condensed Matter and Radiation Sciences Division, Naval Research Laboratory, Washington, D.C. 20375-5000
(Received 25 April 1990)

The degree of polarization of channeling radiation emitted by axially channeled electrons has been calculated using the many-beam method. The polarization was found to be substantial, and to increase monotonically with the channeling angle. The many-beam results are compared with those obtained from the single-string approximation and are found to be significantly different.

I. INTRODUCTION

A charged particle directed into a crystal approximately parallel to one of the crystal axes will be channeled;[1,2] that is, it will experience a force which will "steer" the particle along the direction of the axis. For negatively charged particles, such as electrons (which will be considered in this paper), the channel is provided by the crystal axis.

From a quantum-mechanical viewpoint, the channel is the source of a potential well in the direction transverse to the particle's motion, which gives rise to transversely bound states for the particle. Transitions to lower-energy states lead to the phenomenon known as channeling radiation. The fact that the transverse potential is periodic allows the use of the Bloch-function or "many-beam" approach to this problem. This was first done by Anderson *et al.*[3]

In this paper, we report the results obtained when the Bloch-function approach was used to calculate the polarization of channeling radiation. Numerical results for the case of 4-MeV electrons channeling along the $\langle 100 \rangle$ axis of Si will be presented.

The organization of this paper is as follows. In Sec. II, the quantum-electrodynamic theory of radiation is reviewed and applied to the channeling radiation problem. The many-beam approach to channeling is also presented in this section. In Sec. III, the numerical results for a representative example are given. Finally, conclusions are presented in Sec. IV.

II. THEORY

The quantum-mechanical calculation of axial channeling radiation was first carried out by Kumakhov and Wedell,[4] and the following analysis utilizes their developments. One begins with the time-independent Dirac equation for an electron moving in a potential $V(x,y)$ periodic in the xy plane (which is perpendicular to the direction of the incident electrons):

$$[-i\boldsymbol{\alpha}\cdot\nabla-\beta m+V(\boldsymbol{\rho})]\Phi=E\Phi \ , \tag{1}$$

where m and E are the electron's mass and energy, respectively, $\boldsymbol{\rho}=(x,y)$, $\boldsymbol{\alpha}$ and β are the standard Dirac matrices given by

$$\boldsymbol{\alpha}\equiv\begin{bmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{bmatrix} \tag{2a}$$

and

$$\beta=\begin{bmatrix}I & 0\\ 0 & -I\end{bmatrix} , \tag{2b}$$

and $V(x,y)$ is the average value of $V(x,y,z)$ along z:

$$V(x,y)=\frac{1}{L}\int_0^L V(x,y,z)dz \ . \tag{3}$$

This approximation is valid if the electron is channeled and its energy satisfies the inequality[1]

$$E>2Ze^2\frac{d}{a^2} \ , \tag{4}$$

where Z is the atomic number of the crystal atoms, e is the electron charge, a is the Thomas-Fermi screening length, and d is the distance between atoms along the string. The atomic potentials used in Eq. (3) are of the form given by Doyle and Turner,[5] modified to include the effects of thermal vibration of the lattice atoms.

Separating the wave function into large and small components,

$$\Phi=\begin{bmatrix}\phi_+\\ \phi_-\end{bmatrix} , \tag{5}$$

leads to a Pauli-type equation for the large components:

$$\boldsymbol{\sigma}\cdot\nabla(E-V+m)^{-1}\boldsymbol{\sigma}\cdot\nabla\phi_+ +(E-V-m)\phi_+=0 \ . \tag{6}$$

Since the potential is independent of z, the solution of the wave equation can be written in the form

$$\phi_+\propto\exp(ip_z z)\Psi(\boldsymbol{\rho})\chi \ . \tag{7}$$

One now takes advantage of the fact that the electrons of interest have kinetic energy on the order of 1 MeV, which is much larger than the axial potential energy, which is on the order of 100 eV. This allows one to transform Eq.(6) into a two-dimensional, relativistic Schrödinger

 ©1990 The American Physical Society

equation:

$$\frac{-1}{2\gamma m}\nabla_{x,y}\Psi+V(x,y)\Psi=E_{\perp}\Psi \ , \tag{8}$$

where γ is the relativistic factor and $E_{\perp}$ is the transverse energy of the electron.

Now consider the emission of a photon by the channeled electron. Using quantum electrodynamics,[6] the single-photon spontaneous emission rate is proportional to the square of the radiative-transition matrix element, which is given by

$$\mathbf{j}(\mathbf{k})=\int \Phi_f^{\dagger}(\mathbf{r})\alpha\Phi_i(\mathbf{r})\exp\left[-i\mathbf{k}\cdot\mathbf{r}\right]d^3r \ , \tag{9}$$

where $\mathbf{k}$ is the photon momentum. In the many-beam formulation, the spatial part of the wave function is written as

$$\Psi_{\mathbf{p}_{i(f)}}(\mathbf{r})=\exp\left[i\mathbf{p}_{i(f)}\cdot\mathbf{r}\right]\sum_{\mathbf{g}}c_{\mathbf{g}}\exp\left[i\mathbf{g}\cdot\mathbf{r}\right] \ , \tag{10}$$

where $\mathbf{p}_{i(f)}$ is the initial (final) momentum of the electron and the $\mathbf{g}$ are the reciprocal lattice vectors. When this expression is inserted into the expression for the matrix element [Eq. (9)], the result, neglecting a spin-dependent term, is

$$\mathbf{j}(\mathbf{k})=\frac{1}{\gamma mc}\sum_{\mathbf{g}}c_{\mathbf{g}}c^{*}_{\mathbf{g}+\mathbf{K}}(\mathbf{p}_i+\mathbf{g})\delta(\mathbf{p}_i-\mathbf{p}_f-\mathbf{k}-\mathbf{K}) \ . \tag{11}$$

In order to evaluate the matrix element, one needs the numerical value of the coefficients $c_{\mathbf{g}}$. These are found by solving the wave equation [Eq. (8)] in the many-beam formulation. To do this, one writes the two-dimensional wave function Ψ as

$$\Psi(\boldsymbol{\rho})=\exp\left[i\mathbf{p}_{\perp}\cdot\boldsymbol{\rho}\right]\sum_{\mathbf{g}}c_{\mathbf{g}}\exp\left[i\mathbf{g}\cdot\boldsymbol{\rho}\right] \ , \tag{12a}$$

and the transverse potential as

$$V(\boldsymbol{\rho})=\sum_{\mathbf{g}}V_{\mathbf{g}}\exp\left[i\mathbf{g}\cdot\boldsymbol{\rho}\right] \ . \tag{12b}$$

Substitution of Eqs. (12) into Eq. (8) leads to the linear set of equations

$$\frac{1}{2m\gamma}|\mathbf{p}_{\perp}+\mathbf{g}|^2c_{\mathbf{g}}+\sum_{\mathbf{g}'}c_{\mathbf{g}'}V_{\mathbf{g}-\mathbf{g}'}=E_{\perp}c_{\mathbf{g}} \ , \tag{13}$$

which, when truncated to include a finite number of coefficients, can be solved numerically.

Once the coefficients have been obtained, the emitted photon intensity can be determined. The differential intensity for a given polarization is, by Fermi's Golden Rule,

$$\frac{d^2I_i}{dk\,d\Omega}=\frac{e^2k^2}{2\pi E^2}\delta(k-k\beta_{\parallel}-\omega)|\mathbf{j}\cdot\hat{\boldsymbol{\varepsilon}}_i^{*}|^2 \ , \tag{14}$$

where ω is the energy difference between the two levels in the rest frame of the electron and $\hat{\boldsymbol{\varepsilon}}_i$ are the photon polarization vectors. The photon polarization is given by the difference in intensity for the two polarizations dI_l and dI_2, normalized by the total intensity dI_1+dl_2, as

$$p=\frac{dI_1-dI_2}{dI_1+dI_2} \ . \tag{15}$$

III. RESULTS

The geometry of the problem is shown in Fig. 1. The incident electron momentum makes an angle θ with the z axis and an angle ϕ with the x axis. The emitted photon momentum is taken, in this work, to be parallel to that of the electron, for the purpose of calculating the polarization in the forward direction. The photon polarization vector $\hat{\boldsymbol{\varepsilon}}_1$ makes an angle θ with the x axis and lies in the xz plane, and $\hat{\boldsymbol{\varepsilon}}_2$ is parallel to the y axis. The x and y axes are in the direction of the nearest-neighbor atoms; i.e., they are each parallel to one of the basic transverse reciprocal lattice vectors. In this case (channeling along the $\langle 100\rangle$ axis of Si), the two reciprocal lattice vectors are equal in magnitude.

When the particular polarization vectors which were chosen are inserted into the intensity formula [Eq. (14)], the expression for the polarization becomes

$$p=\frac{\langle j_x\rangle^2\cos^2\theta-\langle j_y\rangle^2}{\langle j_x\rangle^2\cos^2\theta+\langle j_y\rangle^2} \ , \tag{16}$$

where

$$j_x(k_x)=\frac{1}{\gamma mc}\sum_{g_x}c_{g_x}c^{*}_{g_x+K_x}(p_{ix}+g_x)\times\delta(p_{ix}-p_{fx}-k_x-K_x) \tag{17}$$

is the matrix element in the x direction and the expression for j_y is similar. These two matrix elements are, in general, not equal, and this gives rise to a polarization which can be substantial, as shown in Fig. 2. The polarization varies from zero, when the electron is exactly aligned with the z axis, to a maximum which depends on the angle ϕ. The maximum value of θ shown corresponds, approximately, to the critical channeling angle,[1] which is the angle at which the electrons are no longer channeled. Beyond this value, the polarization decreases smoothly to a minimum value of approximately -1, then

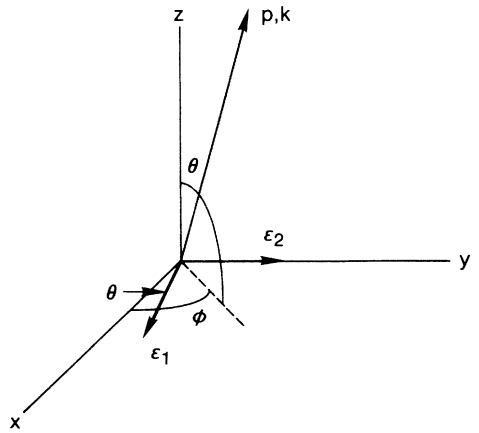

FIG. 1. Geometry of the channeling radiation problem.

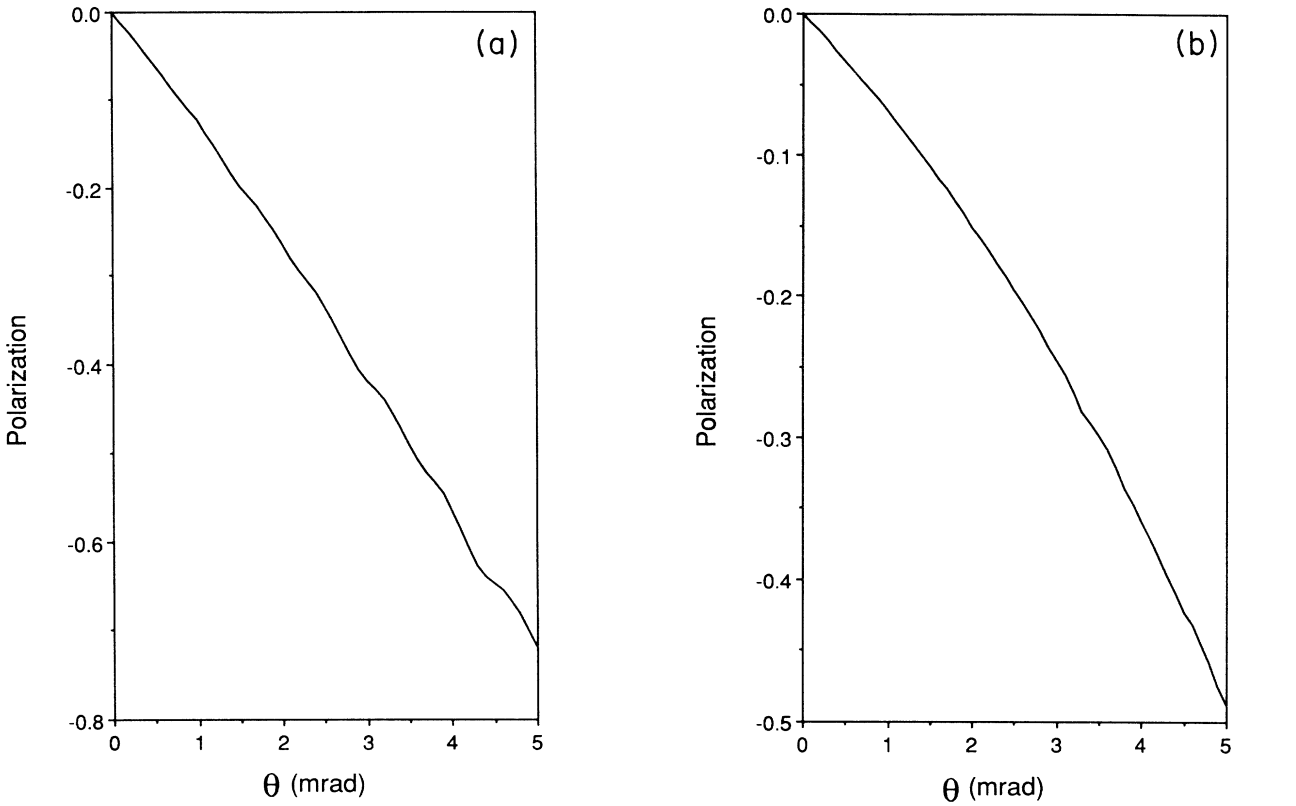

FIG. 2. Polarization of channeling radiation emitted by 4-MeV electrons incident along the ⟨100⟩ axis of Si, during the transition $2p$-$1s$, as a function of the polar angle θ. (a) $\phi=0$. (b) $\phi=\pi/8$.

increases abruptly to zero before an oscillatory motion begins. These results are not shown since the critical channeling angle Ψ_c is approximately the same angle at which the theoretical basis for the continuum model is no longer valid. Although some coherent effects have been observed at angles greater than Ψ_c, the validity of the model used is not obvious at these angles. For this reason, the results for these angles are not presented quantitatively here. Experimental measurement of the polarization of channeling radiation may, then, be a probe of the range of validity of the continuum approximation.

The dependence of the polarization on ϕ is shown in Fig. 3. For a fixed, nonzero, value of θ, the polarization varies from a maximum at $\theta=0$ rad to nearly zero at $\theta=\pi/4$ rad. The values shown are for the transition between the $2p$ and $1s$ states. The results for other transitions are identical. Also, the results for other values of the electron energy are qualitatively the same as those presented here.

Calculations[3] of the band structure and photon intensity for 4-MeV electrons along the ⟨100⟩ and ⟨111⟩ axes of Si have shown that the tight-binding approximation gives very good results for these quantities. The present calculations, however, have shown that it is inadequate for calculations of polarization. The matrix elements in the tight-binding approximation, which uses wave functions calculated in the single-string approximation, are equivalent for the x and y directions. (Alternatively, one

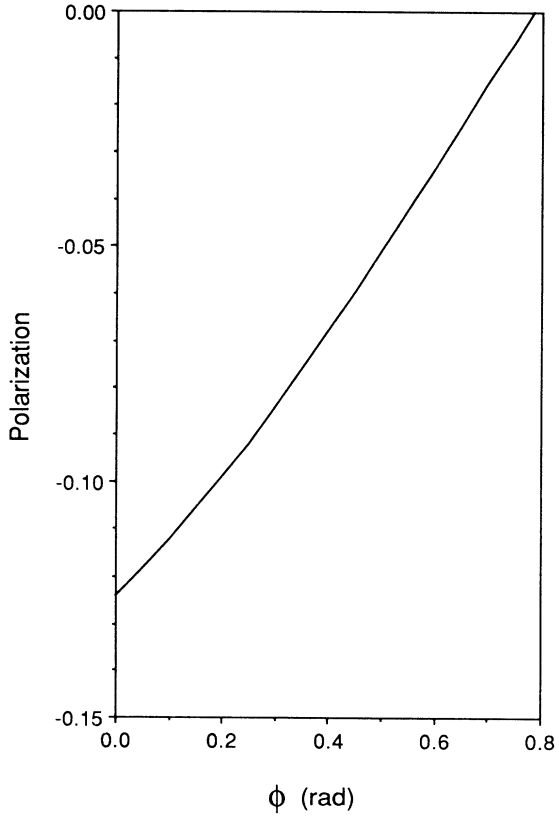

FIG. 3. Polarization as a function of the azimuthal angle ϕ, for $\theta=1$ mrad.

can say that there is only one matrix element, which depends only on ρ, the distance from the string.) The expression for the polarization can then be written simply as

$$P=\frac{\cos^2\theta-1}{\cos^2\theta+1} , \tag{18}$$

which is very small for the values of θ which result in channeling. The many-beam values of the polarization take on this value when the two matrix elements are equal. This occurs when ϕ takes on the values

$$\phi=n\frac{\pi}{4} , \quad n=1,3,\ldots . \tag{19}$$

IV. CONCLUSIONS

The polarization of channeling radiation may be useful in the determination of the crystal potential experienced by a channeled electron[7] and as a source of tunable, narrow-bandwidth, polarized radiation.[8] In this paper, we have calculated the polarization of channeling radiation using the many-beam technique and have found that it is a significant effect. The many-beam results were found to be quite different from those obtained using the tight-binding approximation.

ACKNOWLEDGMENTS

The author wishes to thank A. W. Sáenz and H. Überall for helpful discussions and V. L. Jacobs for his comments on this manuscript. This work was supported by the Office of Naval Research through the Office of Naval Technology.

[1]J. Lindhard, Mat. Fys. Medd. Dansk Vid. Selsk. **34**, 1 (1965).
[2]D. S. Gemmell, Rev. Mod. Phys. **46**, 129 (1974).
[3]J. U. Andersen, E. Bonderup, E. Laegsgaard, B. B. Marsh, and A. H. Sørensen, Nucl. Instrum. Methods **194**, 209 (1982).
[4]M. A. Kumakhov and R. Wedell, Phys. Status Solidi B **84**, 581 (1977).
[5]P. A. Doyle and P. S. Turner, Acta Crystallogr. A **24**, 390 (1968).
[6]V. B. Berestetskii, E. M. Lifshitz, and L. P. Pitaevskii, *Quantum Electrodynamics* (Pergamon, New York, 1982), p. 164.
[7]R. H. Pantell and R. L. Swent, Appl. Phys. Lett. **25**, 910 (1979).
[8]M. A. Kumakhov, Phys. Lett. **57A**, 17 (1976); Dokl. Acad. Nauk SSSR **231**, 1077 (1976) [Sov. Phys. Doklady **21**, 581 (1976)]; Zh. Eksp. Teor. Fiz. **72**, 1489 (1977) [Sov. Phys. JETP **45**, 781 (1977)].