TWO-DIMENSIONAL CALCULATION OF CHANNELING RADIATION SPECTRUM FOR HIGH-BRIGHTNESS HARD X-RAY PRODUCTION

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Abstract

The channeling radiation spectrum is calculated without using the one-dimensional approximation in the planar channeling radiation model or the single-string approximation in the axial channeling radiation model. The obtained spectrum of the two-dimensional channeling radiation is significantly different from those previously calculated with the approximations. The calculation presented here is of the channeling radiation experiments conducted at Fermilab Advanced Superconducting Test Accelerator (ASTA) photoinjector with electron beam energies of 20 to 50 MeV and a diamond target. The computational method developed in this work can be applied to general cases of different crystals and beams with different energy and emittances.

INTRODUCTION

High-energy channeling radiation is produced by a relativistic electron beam interacting with a crystal lattice when the beam channels through the crystal. When an ultra-relativistic electron enters a crystal, the electron will channel through the crystal lattice if its incident angle relative to a specific lattice direction is sufficiently small [1]. A high-intensity ultra-relativistic electron beam could produce high-brightness hard X-rays due to the perturbation of the transverse motion of beam electrons in the crystal. To study this channeling radiation theoretically and numerically, the interaction between the lattice ions and beam electrons has previously been modelled with two different approximations. In the planar channeling approximation [2–4], the radiation from beam electrons is calculated approximately using the Bloch wave function of the electrons solved in a one-dimensional transverse space. In the axial channeling model [2, 5], on the other hand, a single-string approximation of the lattice potential results in a rotational symmetry in the two-dimensional transverse space that greatly simplifies the computational complexity of the original problem of two-dimensional energy bands calculation. Even though these approximations have been justified by the fact that the most relevant energy states for the channeling radiation are those deeply bound states, it is not clear what the conditions are for the validity of the approximations, especially for the case of high-brightness electron beams. In this paper, the channeling radiation spectrum is calculated numerically by solving the Bloch wave function in the two-dimensional transverse space without using the planar or axial channeling approximations. This study is for the upcoming channeling radiation experiments on Fermilab ASTA facility with a 20 to 50 MeV electron beam incident on a diamond lattice along the [-110] lattice direction [6, 7]. In this study, we used a 14.6 MeV electron beam with rms emittance of 0.1 μm in the both transverse directions and the beta functions at the crystal are 4.0 m in the both directions.

LATTICE INTERACTIONAL POTENTIAL IN TRANSVERSE PLANE

When a relativistic beam electron channels through a crystal, the ions of the crystal lattice interact with the electron and affect the motion of the electron. The change of the electron motion results in the emission of photons. Since the longitudinal motion of the electron is ultra-relativistic, the interaction from the ions is too weak to have any effect on the longitudinal motion. The transverse motion of the electron is non-relativistic and the interaction from the ions could have a significant effect on the motion. For the transverse motion, in this study, the interaction potential $V(x, y)$ in the transverse plane is obtained by averaging the lattice potential $V_{cell}(\vec{r})$ in three-dimensional space along the longitudinal direction, where $V_{cell}(\vec{r})$ is the interaction potential of the ions in one unit cell and calculated by using Doyle-Turners formula based on a fitting to the electron scattering factor of the crystal [8]. Due to the periodicity of the lattice in the transverse plane, $V(x, y)$ can be written as a Fourier expansion with the reciprocal lattice vectors projected to the transverse plane. For a beam channeling along the [-110] direction of diamond lattice, the x and y axis of the transverse plane can be chosen to be along the [110] and [001] direction, respectively, and the reciprocal lattice constants of the transverse plane are $b_1 = 2\sqrt{2}\pi/a$ and $b_2 = 2\pi/a$ for the two directions, where a is diamond lattice constant. The interaction potential for the transverse motion of beam electrons can then be written as

$$V(x, y) = \sum_{k_1,k_2=-\infty}^{\infty} V_{k_1,k_2}\, e^{i(k_1 b_1 x + k_2 b_2 y)} \qquad (1)$$

where the expansion coefficients V_{k_1,k_2} are calculated using the formulas given in [5] and the summations of k_1 and k_2 need to be truncated at $\pm k_{max}$ for a numerical solution of the Schrödinger equation of the beam electron in the lattice. In this study, it was found that the convergence of the truncation occurs at $k_{max} = 20$ as the change of $V(x, y)$ due to the additional terms of $k_{max} > 20$ is negligible. Figure 1 plots $V(x, y)$ in a unit cell and shows that the interaction potential in the transverse plane does not have a rotational symmetry of the potential used in the axial channeling approximation. The asymmetry of $V(x, y)$ between the x and y direction is because the two-dimensional lattice in the transverse plane becomes rectanglar as $b_1 \neq b_2$, which results from the projection of the cubic diamond lattice to the transverse plane.

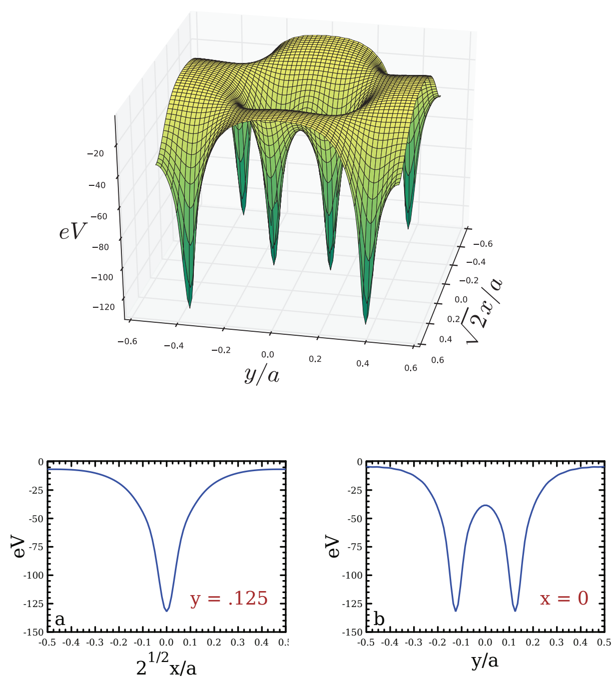

Figure 1: The top figure is $V(x, y)$ for the channeling along the [-110] direction of diamond. The bottom figures are the cross section of $V(x, y)$ at (a) $y = 0.125$ and (b) $x = 0$.

It should also be noted that the potential wells of $V(x, y)$ in the transverse space are about four times deeper than the single potential well in the one-dimensional approximation of the planar channeling model.

ENERGY BANDS

The wave function of the beam electrons in the transverse plane is a Bloch wave that can be expanded into plane waves as

$$\Psi_\Omega(x, y) = \frac{1}{2\pi} \sum_{k_1,k_2} C_{k_1,k_2} e^{i[(k_1+Q_1)b_1x+(k_2+Q_2)b_2y]} \quad (2)$$

where the summations are truncated similar to $V(x, y)$ as k_1 and k_2 are from $-k_{max}$ to k_{max} and $-0.5 \le (Q_1, Q_2) < 0.5$ for the first Brillouin zone. With the truncated plane wave expansion of the Bloch wave, the Schrödinger equation in the rest frame of the beam can be written as

$$\sum_{l_1,l_2} \left\{ \left[(k_1 + Q_1)^2 + \left(\frac{b_2}{b_1}\right)^2 (k_2 + Q_2)^2 \right] \delta_{l_1k_1}\delta_{l_2k_2} + \frac{1}{\epsilon} V_{k_1-l_1,k_2-l_2} \right\} C_{l_1,l_2} = \frac{E_n(\vec{Q})}{\gamma\epsilon} C_{k_1,k_2} \quad (3)$$

where l_1 and l_2 are from $-k_{max}$ to k_{max}, γ is the Lorentz factor of the beam, $\epsilon = \hbar^2 b_1^2/(2\gamma m_e)$ and $E_n(\vec{Q})$ is the eigen energy with the index n numbering the energy bands. This eigen equation can be solved by diagonalization of a $(2k_{max} + 1)^2 \times (2k_{max} + 1)^2$ matrix for each given $\vec{Q} = (Q_1, Q_2)$. Figure 2 plots the probability density $|\Psi_\Omega(x, y)|^2$ of the obtained eigenstates for $n = 0$ and $n = 1$ and clearly shows that $|\Psi_\Omega(x, y)|^2$ is not rotationally symmetric in the transverse plane even at two lowest eigenstates. The rotational symmetry of the density function in the axial channeling model severs the asymmetric feature (the peaks away from $x = y = 0$ in Fig. 2) of the wave function and the justification of the axial channeling approximation is apparently problematic.

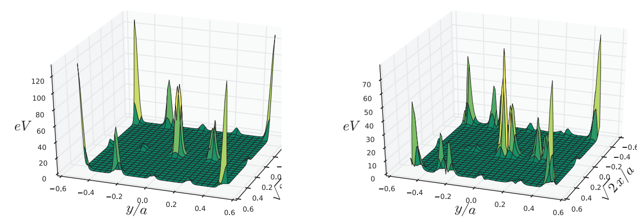

Figure 2: Wave Density function for (a) $n = 0$ and (b) $n = 1$ with $Q_1 = Q_2 = 0$.

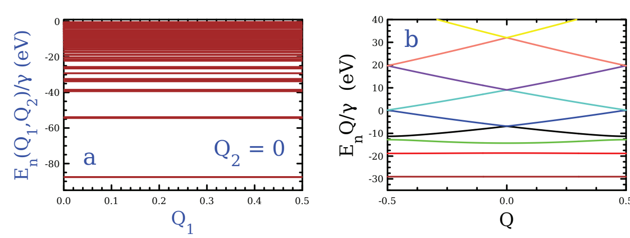

Figure 3: Energy bands in the lab frame of the beam calculated (a) in two-dimensional transverse plane with the potential in Fig. 1 and (b) with one-dimensional planar channeling approximation.

In Fig. 3, the negative energy bands for the channeling along the [-110] direction in diamond are plotted for different values of (Q_1, Q_2). For a comparison, the eigen energies of the same system calculated by using the one-dimensional planar channeling approximation is also included. The energy bands obtained in the two-dimension calculation is very different from the one calculated with one-dimensional approximation. The gaps between the lowest three energy states are larger than those of the one-dimensional calculation. Moreover, in the two-dimensional case, there are 111 negative eigen energy states while in the one-dimensional planar channeling, there are only 6 negative eigen energy states. The much richer energy band in the two-dimensional case is apparently due to a much deeper and more complex interaction potential in the two dimensional case.

RADIATION SPECTRUM

The selection matrix for the electron transition from the energy eigen state of $(n, \vec{Q})$ to another state of $(m, \vec{Q}\,')$ due

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to the perturbation $H_1' = \epsilon \vec{A} \cdot \vec{p}$ can be calculated as

$$\left|\left\langle \vec{Q}', m \left| H_1 \right| \vec{Q}, n \right\rangle\right|^2 = d_0 \mathcal{T}(n, \vec{Q}, m, \vec{Q})\, \delta(\vec{Q} - \vec{Q}') \quad (4)$$

where d_0 is a constant that is independent of eigen states and

$$\mathcal{T}(n, \vec{Q}, m, \vec{Q}) = \left\{ \sum_{k_1, k_2} C_{k_1,k_2}(\vec{Q}, n)\, C^*_{k_1,k_2}(\vec{Q}, m) \right. \\ \left. \times \left[(k_1 + Q_1) + \frac{b_2}{b_1}(k_2 + Q_2) \right] \right\}^2 \quad (5)$$

For a beam distribution in the transverse momentum space

$$f(p_x) = \frac{1}{2\pi\sigma_x\sigma_y} e^{-p_x^2/(2\sigma_x^2) - p_y^2/(2\sigma_y^2)} \quad (6)$$

the occupation probability of the beam electrons on the eigen-state of $(n, \vec{Q})$ can be calculated as

$$\mathcal{N}(n, \vec{Q}) = \frac{h^2 b_1 b_2}{\sqrt{2\pi}\sigma_x\sigma_y} \int_{-P_{1,max}}^{P_{1,max}} \int_{-P_{2,max}}^{P_{2,max}} \quad (7) \\ \left| C_{k_1,k_2}(\vec{Q}, n) \right|^2_{\vec{P} = \vec{k} + \vec{Q}} e^{-P_1^2/(2\sigma_{kx}^2) - P_2^2/(2\sigma_{ky}^2)}\, dP_1\, dP_2$$

where $\sigma_{kx} = \sigma_x (hb_1)^{-1}$, $\sigma_{ky} = \sigma_y (hb_2)^{-1}$, $P_{i,max} = p_{max}(hb_i)^{-1}$, $p_{max} = (2\gamma m_e |min(V(x,y))|)^{1/2}$ is the maximum transverse momentum for the channeling, and the integration over $\vec{P}$ can be evaluated numerically.

The radiation intensity for the transition from the eigen state of $(n, \vec{Q})$ to the state of $(m, \vec{Q}\,')$ can then be calculated as

$$\mathcal{N}(n, \vec{Q})\, \mathcal{T}(n, \vec{Q}, m, \vec{Q})\, \delta(\vec{Q}' - \vec{Q})$$

Since the ground state ($m = 0$) energy is independent of $\vec{Q}$, for the transition to the ground state we should account all the transitions to $m = 0$ states with any $\vec{Q}$. The overall radiation intensity to the ground state is thus proportional

$$\text{Radiation Intensity} = \int \mathcal{N}(n, \vec{Q})\, \mathcal{T}(n, \vec{Q}, 0, \vec{Q})\, d\vec{Q} \quad (8)$$

Figure 4 plots the radiation spectrum in Lab frame of 14.6 MeV electron beam channeling through diamond lattice along the [-110] direction calculated using Eq. (8) and, for a comparison, it also includes the same spectrum calculated using the planar channeling approximation. The spectrum obtained with the full two-dimensional calculation (Fig. 4a) has two dominate peaks at ~ 55 and 110 keV which are missing from the one-dimensional calculation (Fig. 4b). Most peaks in the spectrum of the one-dimensional calculation are, on the other hand, present in the spectrum of the two-dimensional calculation. The difference between the two spectrum is significant, especially at radiation energy higher than 40 keV in this case. Those radiations peaks with higher energy could be preferred for the design of high-brightness hard X-ray sources.

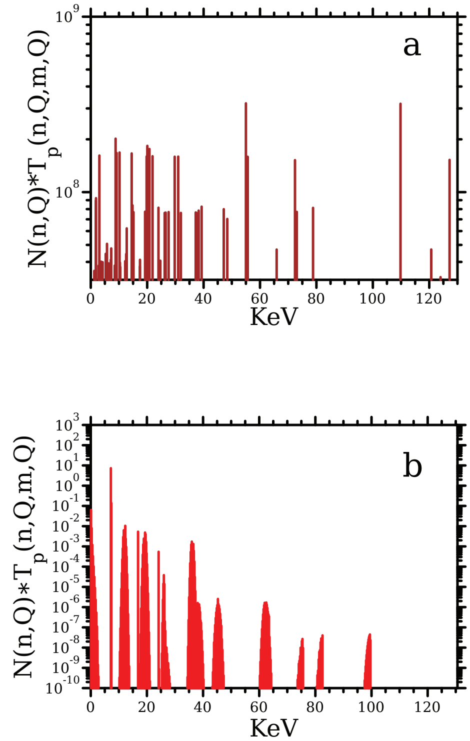

Figure 4: Radiation spectrum in Lab frame of 14.6 MeV beam channeling along the [-110] direction of diamond calculated (a) with the full two-dimensional model and (b) with planar channeling approximation.

CONCLUSION

The planar and axial model of channeling radiation provide clear geometrical descriptions and easy computational approaches for studying channeling radiation. Their limitations due to the approximations involved could, however, be significant as shown in this study. The full two-dimensional calculation of the energy band provides a more complete spectrum for channeling radiation.

REFERENCES

[1] J. Lindhard, Phys. Lett. **12**, 126 (1964).

[2] K. Chouffani and H. Uberall, Phys. Stat. Sol. B**213**, 107 (1999).

[3] B. Azadegan, et al, Phys. Rev. B**74**, 045209 (2006).

[4] B. Azadegan, Comp. phys. Commu. **184**, 1064 (2013).

[5] J.U. Andersen et al, Nucl. Instrum. Meth. & Inst. **194**, 209 (1982).

[6] T. Sen and C. Lynn, FERMILAB-PUB-14-243-APC.

[7] P. Piot et al, FERMILAB-CONF-13-086-AD-APC.

[8] P.A. Doyle and P.S. Turner, Acta Cryst. A**24**, 390 (1968).