A general formalism of two-dimensional lattice potential on beam transverse plane for studying channeling radiation

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Abstract

To study channeling radiation produced by an ultra-relativistic electron beam channeling through a single crystal, a lattice potential of the crystal is required for solving the transverse motion of beam electrons under the influence of the crystal lattice. In this paper, we present a general formalism for this two-dimensional lattice potential of a crystal with a Lorentz contraction in the beam channeling direction. With this formalism, the lattice potential can be calculated without approximation from any given model of electron-ion interaction for an ultra-relativistic beam channeling in any crystal direction. The formalism presented should be the standard recipe of the lattice potential for studying the channeling radiation.
There has been a renewed interest recently in channeling radiation produced from an electron beam interacting with a crystal lattice for its potential application in hard X-ray production. When an ultra-relativistic electron enters a single crystal, rather than having random scattering, the electron will channel through the crystal lattice if its incident angle relative to a specific lattice orientation of the crystal is sufficiently small. During the channeling, the non-relativistic motion of the electron in the transverse plane that is perpendicular to the channeling direction could be strongly perturbed by the crystal lattice while the ultra-relativistic motion of the electron along the channeling direction is unperturbed. 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 a crystal.

The channeling radiation is considered to be from the transitions between bounded Bloch eigenstates for the transverse motion of beam electrons during the channeling. To study the radiation theoretically and numerically, the interaction between the crystal lattice and beam electrons has been modeled in two different approaches, the one-dimensional (1D) planar and the two-dimensional (2D) axial channeling model. In the planar channeling model, the transverse motion of the electrons is assumed to be aligned in a single crystal direction during the channeling and the Bloch eigenstates for the transverse motion are solved from a 1D Schrödinger equation. This 1D approximation is valid only if the coupling between the original 2D motion of the electrons in the transverse plane is negligible. Note that the lattice potential for the transverse motion of the channeling electrons is the result of a Lorentz contraction of the three-dimensional (3D) crystal lattice in the beam rest frame where the crystal travels with near the speed of light along (opposite to) the beam channeling direction and the 3D crystal lattice is pancaked into a 2D lattice on the beam transverse plane. The resulting lattice potential is strongly coupled in the 2D transverse plane and the transverse motion of a channeling electron in a crystal cannot be decoupled into 1D motion if the lattice potential dominates the Hamiltonian. At the bounded Bloch eigenstates for the channeling radiation, the transverse energy is negative (inside lattice potential wells) and the lattice potential dominates the transverse kinetic energy. Therefore, the 1D approximation of the planar channeling model cannot be justified rigorously and the study of the channeling radiation should be based on the Bloch eigenstates.
for the 2D transverse motion of beam electrons in a crystal. In order to solve the Bloch eigenstates in the 2D transverse plane, a lattice potential in the transverse plane is required. To obtain this potential of the 2D lattice, in the axial channeling model, the ions in the original crystal are first grouped into strings of the ions along the channeling direction and the lattice potential is calculated by summing up the contributions of the strings of the ions \([15, 16, 18]\). In this direct calculation of the lattice potential, the identification of the strings of the ions and the summation over the strings are cumbersome and, in some cases, difficult due to a complicated geometric relationship among lattice ions along the channeling direction. Moreover, the calculation with the strings of the ions has to be specifically tailored for each specific crystal structure and channeling direction, which can hardly be applied to other cases because of the difference in the strings of the ions with different crystal structure and different channeling direction.

An accurate lattice potential on the transverse plane is necessary for calculating the Bloch eigenstates of the 2D transverse motion of beam electrons in a crystal. With a given interaction between a beam electron and individual ion in a crystal, such as the Born approximation for electron scattering from an ion with Doyle-Turner fitting parameters \([19]\), the question is what is the best approach, in terms of accuracy, mathematical simplicity, and general applicability to any crystal structure and channeling direction, for the construction of the lattice potential on the 2D transverse plane. In this paper, we present a new and better approach for this 2D lattice potential calculation. In this new approach, a lattice potential of the original three-dimensional crystal is first calculated from a given electron-ion interaction potential in the original unit cell coordinate of the crystal by taking the advantage of the native periodicity of the crystal lattice. This potential of the three-dimensional lattice in the unit-cell coordinate is then transferred into the beam coordinate that is aligned with the beam longitudinal (channeling) and transverse directions using rotational coordinate transformations. Lastly, the Lorentz contraction of the lattice can be easily accomplished mathematically by averaging the three-dimensional lattice potential in the beam coordinate along the channeling direction. In this approach, the calculation of the lattice potential is mathematically clean, systematic, and can be easily applied to any crystal with any channeling direction. This generic formulation of the 2D lattice potential is developed in Section II, Section III presents several examples of the channeling in different crystal direction, and Section IV contains a final remarks.
II. FORMULATION OF LATTICE POTENTIAL IN BEAM TRANSVERSE PLANE

When an ultra-relativistic electron beam channels through a crystal lattice with a specific orientation aligned along the beam longitudinal direction, the non-relativistic transverse motion of the electrons is perturbed by the lattice of ions in the crystal. To formulate this lattice potential, we consider an orthorhombic crystal lattice with each unit cell of the lattice containing $N$ ions. Let $\vec{r}_j$ with $j = 1, \ldots, N$ be the local coordinates of the ions in a unit cell, where the origin of the local coordinate is at a corner of a unit cell, and $\vec{r}_m = (m_1a_1, m_2a_2, m_3a_3)$ be the global coordinate of a unit cell, where $(a_1, a_2, a_3)$ are lattice constants of the crystal and $\vec{m} = (m_1, m_2, m_3)$ are an integer vector. Let $\vec{X} = (X_1, X_2, X_3)$ be a global coordinate, referred as lattice coordinate, with the axes of $X_1$, $X_2$, and $X_3$ aligned with the primary crystal axes along [100], [010], and [001] crystal direction, respectively. When an electron travels through the crystal, the interaction between the electron and the crystal lattice can be calculated by a superposition of the interactions between the electron and each individual ion as

$$V_{3D}(\vec{X}) = \sum_{\vec{m}=-\infty}^{\infty} \sum_{j=1}^{N} V_{\text{ion}}(\vec{X} - \vec{r}_m - \vec{r}_j)$$

(1)

where $V_{\text{ion}}(\vec{r})$ is the interaction potential between an electron and a single ion in the crystal. Note that $V_{3D}(\vec{X})$ is periodic in the crystal, i.e. $V_{3D}(\vec{X} + \vec{r}_l) = V_{3D}(\vec{X})$, where $\vec{r}_l = (l_1a_1, l_2a_2, l_3a_3)$ and $(l_1, l_2, l_3)$ is any combination of integers. With the lattice native periodicity $(a_1, a_2, a_3)$, $V_{3D}(\vec{X})$ can be rewritten into a Fourier expansion of

$$V_{3D}(\vec{X}) = \sum_{\vec{k}=-\infty}^{\infty} V_{\vec{k}} e^{i\vec{G} \cdot \vec{X}}$$

(2)

where $\vec{G} = 2\pi(k_1/a_1, k_2/a_2, k_3/a_3)$ is the reciprocal lattice vector of the crystal. The Fourier expansion coefficient $V_{\vec{k}}$ can be calculated as

$$V_{\vec{k}} = \frac{1}{a_1a_2a_3} \sum_{\vec{m}=-\infty}^{\infty} \sum_{j=1}^{N} \int_{0}^{a_1} \int_{0}^{a_2} \int_{0}^{a_3} V_{\text{ion}}(\vec{X} - \vec{r}_m - \vec{r}_j) e^{-i\vec{G} \cdot \vec{X}} d\vec{X}$$

$$= \frac{1}{a_1a_2a_3} \sum_{j=1}^{N} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} V_{\text{ion}}(\vec{\xi} - \vec{r}_j) e^{-i\vec{G} \cdot \vec{\xi}} d\vec{\xi}$$

$$= -\frac{2\pi \hbar^2}{m_e v_0} f_{\text{ion}}(G) \sum_{j=1}^{N} e^{-i\vec{G} \cdot \vec{r}_j}$$

(3)
where $v_0 = a_1 a_2 a_3$ is the unit-cell volume of the crystal, $m_e$ is the electron rest mass, and

$$f_{\text{ion}}(\vec{G}) = -\frac{m_e}{2\pi \hbar^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} V_{\text{ion}}(\vec{\xi}) e^{-i\vec{G} \cdot \vec{\xi}} d\vec{\xi}$$

is the atomic form factor of a single ion in the crystal \[20\]. Note that the lattice potential calculated from Eqs. (3) and (4) includes exactly all the contributions of ions in a crystal and only approximation involved is in the modeling of the electron-ion interaction $V_{\text{ion}}$. With the Doyle-Turner approximation of the form factor \[19\], the electron-ion interaction potential can be expressed as \[15\]

$$V_{\text{ion}}(\vec{\xi}) = -\frac{16\pi^2 \hbar^2}{m_e} \sum_{i=1}^{M} \frac{\alpha_i}{(\beta_i/\pi)^{3/2}} e^{-4\pi^2 |\vec{\xi}|^2/\beta_i}$$

where $\alpha_i$ and $\beta_i$ with $i = 1, \cdots, M$ are the parameters for fitting $f_{\text{ion}}(\vec{G})$ to the relativistic Hartree-Fock calculation of the form factor at values of $|\vec{G}| [19]$. In the original Doyle-Turner’s calculation, four Gaussian functions ($M = 4$) were used in Eq. [20\]. To improve the accuracy at relatively large value of $|\vec{G}|$, Chouffani and Überall used six Gaussian functions ($M = 6$) for the fitting. The obtained values of $\alpha_i$ and $\beta_i$ for diamond, silicon and germanium were given in Ref. [18]. With the electron-ion interaction potential in Eq. (5), the Fourier transformation of the lattice potential of a three-dimensional crystal can then be calculated from Eqs. (3) and (4) as

$$V_{\vec{k}} = -\frac{2\pi \hbar^2}{m_e v_0} \sum_{i=1}^{M} \alpha_i e^{-\lambda_i^2 |\vec{k}|^2/(2a)^2} \sum_{j=1}^{N} e^{-i2\pi(\vec{k} \cdot \vec{r}_j)/a}$$

where $\lambda_i^2 = \beta_i$ for $V_{\text{ion}}$ given in Eq. (5) and $\lambda_i^2 = \beta_i + 8\pi^2 \langle \mu^2 \rangle$ for including the effect of thermal vibrations of the lattice with $\sqrt{\langle \mu^2 \rangle}$ being the root-mean-square displacement of the thermal vibration of the lattice \[15\].

The lattice potential $V_{3D}(\vec{X})$ in Eq. (2) is expressed in the lattice coordinate that is aligned with the primary crystal axes but not aligned with the beam channeling direction. In order to study channeling radiation that is generated from the perturbation of the transverse motion of beam electrons under the influence of the lattice potential, the lattice potential in the beam transverse plane is needed. Since the beam is ultra-relativistic, the interaction between a beam electron channeling through the crystal and the ions in the crystal is too weak to have a significant effect on the longitudinal motion of the electron.
The dependence of the lattice potential on the longitudinal coordinate of the electron can therefore be neglected by averaging the potential over the longitudinal direction. It is thus necessary to transform the lattice potential into a beam coordinate that is aligned with the beam channeling direction. Physically, this is just rotating the crystal lattice so that the crystal axis for the channeling is aligned with the beam direction. Let \( \vec{r} = (x, y, z) \) be the beam coordinate where \( z \) is along the beam channeling (longitudinal) direction of the beam and \( (x, y) \) are two orthogonal coordinates in the beam transverse plane. The transformation from the lattice coordinate \( \vec{X} \) to the beam coordinate \( \vec{r} \) can be accomplished by a \( 3 \times 3 \) rotational matrix \( \mathbf{R} \), \( \vec{r} = \mathbf{R} \vec{X} \). For a beam channeling along the \( [hkl] \) crystal direction, where three integers \( h \), \( k \), and \( l \) are the Miller indices of crystal lattices \([20]\), \( \mathbf{R} \) can be in general constructed with three consecutive transformations (see Fig. 1 for an illustration). The first transformation rotates the lattice coordinate \( (X_1, X_2, X_3) \) in the \( X_1 - X_2 \) plane by an angle of \( \theta_1 = \arctan(k/h) \) and the transformed coordinate is labeled as \( (X'_1, X'_2, X_3) \). The axes of \( X'_1 \) and \( X'_2 \) are aligned with the \( [hk0] \) and \( [\bar{k}h0] \) crystal direction, respectively (see Fig. 1b). The second transformation is rotating \( (X'_1, X'_2, X_3) \) in the \( X'_1 - X_3 \) plane by an angle of \( \theta_2 = \arctan(l/\sqrt{h^2+k^2}) \) and the transformed coordinate is labeled as \( (X''_1, X'_2, X'_3) \). The axes of \( X''_1 \), \( X'_2 \), and \( X'_3 \) are aligned with \( [hkl] \), \( [\bar{k}h0] \), and \( [h_yk_yl_y] \) direction, respectively, (see Fig. 1c) where

\[
(h_y, k_y, l_y) = (h, k, l) \times (-k, h, 0) = (-hl, -kl, h^2 + k^2)
\]

The third transformation is to switch the coordinate axes such that \( x = X'_2 \), \( y = X'_3 \), and \( z = X''_1 \), where \( z \) along the \( [hkl] \) direction is the beam longitudinal coordinate (channeling direction) and \( x \) along the \( [\bar{k}h0] \) direction and \( y \) along the \( [h_yk_yl_y] \) direction are two orthogonal coordinates in the beam transverse plane, respectively. These three coordinate transformations can be expressed as

\[
\vec{X} = \mathbf{R}^{-1} \vec{r} = 
\begin{pmatrix}
\cos \theta_1 & -\sin \theta_1 & 0 \\
\sin \theta_1 & \cos \theta_1 & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\cos \theta_2 & 0 & -\sin \theta_2 \\
0 & 1 & 0 \\
\sin \theta_2 & 0 & \cos \theta_2
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 1 \\
0 & 1 & 0 \\
0 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
\]

(8)

With the transformation matrix \( \mathbf{R} \) in Eq. (8), 3D lattice potential \( V_{3D}(\vec{X}) \) in Eq. (2) can be expressed in the beam coordinate as

\[
V_{3D}(\mathbf{R}^{-1} \vec{r}) = \sum_{\vec{k}=-\infty}^{\infty} V_{\vec{k}} \exp \left[ i(\vec{G}_\mathbf{R} \mathbf{R}^{-1}) \cdot \vec{r} \right]
\]

(9)
where $\vec{G}^T = 2\pi(k_1/a_1, k_2/a_2, k_3/a_3)$ denotes the row vector of $\vec{G}$ for the matrix multiplication. Since the crystal lattice has also periodicities along the orientations of the beam coordinate, $V_{3D}$ is periodic in $\vec{r}$. Let $(b_1, b_2, b_3)$ be the periodicities of the lattice along the $(x, y, z)$ direction, respectively. The periodicity of $V_{3D}(\vec{r})$ requires

$$e^{ib_1(\vec{G}^T\vec{R}^{-1})_1} = e^{ib_2(\vec{G}^T\vec{R}^{-1})_2} = e^{ib_3(\vec{G}^T\vec{R}^{-1})_3} = 1$$

which yields a transformation of the reciprocal lattice vector

$$\left( \frac{k_1}{a_1}, \frac{k_2}{a_2}, \frac{k_3}{a_3} \right) \vec{R}^{-1} = \left( \frac{n_1}{b_1}, \frac{n_2}{b_2}, \frac{n_3}{b_3} \right)$$

(10)

where $(n_1, n_2, n_3)$ are integers. The relationships between $(b_1, b_2, b_3)$ and $(a_1, a_2, a_3)$ and between $(n_1, n_2, n_3)$ and $(k_1, k_2, k_3)$ can be obtained from Eq. (10) with the condition that both $(n_1, n_2, n_3)$ and $(k_1, k_2, k_3)$ are integers for a set of smallest values of $(b_1, b_2, b_3)$. Since the transformation in Eq. (9) is from the expansion in $\vec{X}$ with $(k_1, k_2, k_3)$ as the indices to an expansion in $\vec{r}$ with $(n_1, n_2, n_3)$ as the indices, $(k_1, k_2, k_3)$ as functions of $(n_1, n_2, n_3)$ are needed here. For each given set of $(n_1, n_2, n_3)$ in integers, therefore, $(k_1, k_2, k_3)$ have to be solved from Eq. (10) as integers. With the coordinate of the 3D lattice potential of a crystal correctly aligned with the beam directions, the average of the lattice potential along the beam channeling $(z)$ direction can easily be calculated as

$$V_{2D}(x, y) = \frac{1}{b_3} \int_0^{b_3} V_{3D}(\vec{R}^{-1}\vec{r}) \, dz = \sum_{\vec{k}=-\infty}^{\infty} V_{\vec{k}} e^{i2\pi(n_1x/b_1+n_2y/b_2)} \delta_{n_30}$$

(11)

where $\delta_{n_30}$ is the Kronecker delta for $n_3 = 0$. The Fourier expansion of this projected lattice potential on the transverse plane can then be written as

$$V_{2D}(x, y) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} V_{n_1n_2} e^{i2\pi(n_1x/b_1+n_2y/b_2)}$$

(12)

and the expansion coefficient can be obtained from $V_{\vec{k}}$ of the 3D lattice potential that is calculated using Eqs. (3) and (4) as

$$V_{n_1n_2} = \sum_{\vec{k}=-\infty}^{\infty} V_{\vec{k}} \delta\left(\vec{k} - \vec{k}_0(n_1, n_2)\right)$$

(13)

where $\vec{k}_0(n_1, n_2)$ is the solution of $\vec{k} = (k_1, k_2, k_3)$ as functions of $(n_1, n_2, n_3)$ solved from Eq. (10) with $n_3 = 0$ and the delta functions are the Kronecker delta for $\vec{k} = \vec{k}_0(n_1, n_2)$. 

It should be noted that the minima (potential wells) of \( V_{2D}(x, y) \) in the transverse plane form periodically a 2D lattice that results from the projection of the original crystal lattice onto the transverse plane. The Lorentz contraction along the channeling direction of a three-dimensional lattice can create a more condense structure of ions in the transverse plane. The periodicity of \( V_{2D}(x, y) \) could be smaller than \( b_1 \) and \( b_2 \) due to the averaging of 3D lattice potential \( V_{3D} \) along the beam channeling direction. Mathematically, the change of the periodicity occurs when the summation over the ions in a unit cell in Eq. (6) zeros periodically for certain combinations of \( (k_1, k_2, k_3) \) with \( n_3(\vec{k}) = 0 \). If that occurs, the summation for the Fourier expansion of \( V_{2D}(x, y) \) in Eq. (12) can be rearranged with the correct values of the periods. To solve the Bloch eigenstates for the transverse motion of beam electrons, moreover, one needs to identify the primitive unit cell of the 2D lattice of \( V_{2D}(x, y) \) and the \( x \) and \( y \) coordinate should be aligned with the axes of the primitive unit cell [20]. The crystal axes of the primitive unit cell and the lattice constants that are the periods of \( V_{2D}(x, y) \) can be easily identified by examining the contour plot of \( V_{2D}(x, y) \). If the coordinate \( (x, y) \) in Eq. (12) is not aligned with the primitive unit cell, an additional rotational transformation in the transverse plane is needed for \( V_{2D}(x, y) \).

### III. EXAMPLES

To illustrate this general method for the lattice potential in the beam transverse plane, the potential is calculated for the channeling along [001], [110], [111], and [210] direction of a cubic crystal with a diamond-like atomic structure that has eight ions in a unit cell (e.g. diamond, silicon, germanium). The coordinate of the ions in a unit cell is listed in Table I and the lattice constant of the crystal is denoted by \( a_1 = a_2 = a_3 = a \). For the electron-ion interaction \( V_{ion}(\vec{r}) \), Eq. (6) of the Doyle-Turner model is used in the calculation. All figures for the calculated \( V_{2D}(x, y) \) are plotted with germanium (Ge) lattice and the fitting parameters in the Doyle-Turner model obtained by Chouffani and Überall [18]. For the convenience of reading, those fitting parameters are re-listed in Table II. The value used for the root-mean-square amplitude of the lattice thermal vibration of Ge in Eq. (6) is \( \sqrt{\langle \mu^2 \rangle} = 0.085\text{Å} \) at a temperature of 293 K [21]. The lattice constant of Ge is \( a = 5.658\text{Å} \).
a. Channeling along [001] Crystal Axis

For the channeling along the [001] crystal axis, the beam longitudinal coordinate \( z \) is aligned with the lattice coordinate \( X_3 \). A simple choice of the transverse coordinate is \( x \) and \( y \) aligned with [100] and [010] crystal direction, respectively, and the beam coordinate \((x, y, z)\) is aligned with the lattice coordinate \((X_1, X_2, X_3)\). In Eq. (8), on the other hand, \( \theta_1 = 0 \) and \( \theta_2 = \pi/2 \) for \([hkl] = [001]\), which yields a transformation matrix \( R \) that switches only the \( x \) and \( y \) coordinate and has no any physical consequence on the Fourier transformation of the lattice potential. No coordinate transformation is therefore needed, i.e. \( R \) can be chosen as an identity matrix and the lattice potential \( V_{2D}(x, y) \) can easily be calculated from Eqs. (6) and (13). In the contour plot of the calculated \( V_{2D}(x, y) \), however, the axes of the primitive unit cell of the two-dimensional lattice on the transverse plane were observed to be aligned with the [110] and [\bar{1}10] crystal direction. A rotational transformation in the transverse plane is therefore needed to align \( x \) and the \( y \) axes with the [110] and [\bar{1}10] crystal direction, respectively, i.e.

\[
\begin{pmatrix}
X_1 \\
X_2 \\
X_3
\end{pmatrix} =
\begin{pmatrix}
\cos(\pi/4) & -\sin(\pi/4) & 0 \\
\sin(\pi/4) & \cos(\pi/4) & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix} = R^{-1}
\begin{pmatrix}
x \\
y \\
z
\end{pmatrix}
\]

(14)

where \( \pi/4 \) is the rotation angle from the [100] and [010] direction to the [110] and [\bar{1}10] direction. From Eq. (10), the transformation of the reciprocal lattice vector is

\[
\left(\frac{k_1 + k_2}{\sqrt{2}a}, \frac{k_2 - k_1}{\sqrt{2}a}, \frac{k_3}{a}\right) = \left(\frac{n_1}{b_1}, \frac{n_2}{b_2}, \frac{n_3}{b_3}\right)
\]

(15)

Since for each given set of integers \((n_1, n_2, n_3)\), \((k_1, k_2, k_3)\) have to be solved from Eq. (15) as integers, the solution with the minimal values of \((b_1, b_2, b_3)\) is

\[
\begin{cases}
(b_1, b_2, b_3) = (\sqrt{2}a/2, \sqrt{2}a/2, a) \\
(k_1, k_2, k_3) = (n_1 - n_2, n_1 + n_2, n_3)
\end{cases}
\]

(16)

The lattice potential with \( x \) and \( y \) coordinate aligned with the [110] and [\bar{1}10] crystal axes is then calculated from Eqs. (12), (13), and (6) as

\[
V_{2D}(x, y) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} V_{n_1n_2} \exp \left[ i2\pi \left( \frac{n_1x}{a/\sqrt{2}} + \frac{n_2y}{a/\sqrt{2}} \right) \right]
\]

(17)
where

\[ V_{n_1n_2} = -\frac{2\pi \hbar^2}{m_e v_0} \sum_k \left( \sum_{i=1}^M \alpha_i e^{-\lambda_i^2|\vec{r}_j|^2/(2a^2)} \sum_{j=1}^N e^{-i2\pi(\vec{k}\cdot\vec{r}_j)/a} \right) \delta_{k_1,(n_1-n_2)} \delta_{k_2,(n_1+n_2)} \delta_{k_3,0} \]

\[ = -\frac{2\pi \hbar^2}{m_e a^2} \sum_{i=1}^M \alpha_i e^{-\lambda_i^2(n_1^2+n_2^2)/2a^2} \sum_{j=1}^N e^{-i2\pi[n_1(x_j+y_j)-n_2(x_j-y_j)]/a} \]

(18)

With the coordinate \( \vec{r}_j \) of the ions in a unit cell given in Table I, the second summation in Eq. (18) can be evaluated as

\[ \sum_{j=1}^N e^{-i2\pi[n_1(x_j+y_j)-n_2(x_j-y_j)]/a} = \begin{cases} 8, & \text{for } (n_1, n_2) = (\text{even}, \text{even}) \\ 0, & \text{otherwise} \end{cases} \]

(19)

To purge the terms of zero in the summation of Eq. (17), let \( n_1 = 2k_1 \) and \( n_2 = 2k_2 \), and the lattice potential in the transverse plane can be rewritten as

\[ V_{2D}(x, y) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} v_{k_1k_2} \exp \left[ i\frac{2\pi}{a/(2\sqrt{2})} (k_1x + k_2y) \right] \]

(20)

where

\[ v_{k_1k_2} = V(2k_1)(2k_2) = -\frac{16\pi \hbar^2}{m_e a^2} \sum_{i=1}^M \alpha_i e^{-2\lambda_i^2(k_1^2+k_2^2)/a^2} \]

(21)

The periods of \( V_{2D}(x, y) \) is therefore \( a_x = a_y = a/(2\sqrt{2}) \) in both \( x \) and \( y \) direction when \( x \) and \( y \) axes are aligned with the [110] and [110] crystal axis that are of the primitive cell in the transverse plane of a beam channeling in the [001] direction. The lattice potential in Eqs. (20) and (21) has also been obtained previously using the method of strings of ions in the axial channeling model [18], as this is the easiest case for the axial channeling calculation. As shown in Fig. 2a, \( V_{2D}(x, y) \) has a single potential well in each square unit cell on the beam transverse plane. Near the bottom of the potential wells, where the strings of ions is located, the interaction is almost rotationally symmetric on the transverse plane. The rotational symmetry of the lattice potential has been previously used to simplifying the study of the Bloch eigenstates and transitions between the eigenstates for the transverse motion of beam electrons [12, 16–18].

b. Channeling along [110] Crystal Axis

For a beam channeling in \([hkl] = [110]\) direction, \( \theta_1 = \arctan(k/h) = \pi/4 \) and \( \theta_2 = 0 \) for transformation matrix \( R \) in Eq. (8) and \( h_y = k_y = 0 \) and \( l_y = 2 \) for the Miller indices of the
crystal directions on the transverse plane. The $x$ and $y$ coordinate on the transverse plane are therefore aligned with $[khl] = [1\overline{1}0]$ and $[h_y k_y l_y] = [001]$ crystal axes, respectively. The transformation of the reciprocal lattice vector is calculated from Eq. (10) as

$$
\left( \frac{k_2 - k_1}{\sqrt{2} a} , \frac{k_3}{a} , \frac{k_1 + k_2}{\sqrt{2} a} \right) = \left( \frac{n_1}{b_1} , \frac{n_2}{b_2} , \frac{n_3}{b_3} \right)
$$

For integer $(k_1, k_2, k_3)$ and $(n_1, n_2, n_3)$, the solution of Eq. (22) with the minimal values of $(b_1, b_2, b_3)$ is

$$
\begin{cases}
(b_1, b_2, b_3) = \left( \sqrt{2} a/2 , a , \sqrt{2} a/2 \right) \\
(k_1, k_2, k_3) = (n_3 - n_1, n_1 + n_3, n_2)
\end{cases}
$$

The lattice potential with $x$ and $y$ coordinate aligned with the $[\overline{1}10]$ and $[001]$ crystal axes is then calculated from Eqs. (12), (13), and (6) as

$$
V_{2D}(x, y) = \sum_{n_1=\infty}^{\infty} \sum_{n_2=\infty}^{\infty} V_{n_1n_2} \exp \left[ i2\pi \left( \frac{n_1 x}{a/\sqrt{2}} + \frac{n_2 y}{a} \right) \right]
$$

and

$$
V_{n_1n_2} = -\frac{2\pi \overline{h}^2}{m_e a^2} \sum_{i=1}^{M} \frac{\alpha_i}{\alpha} e^{-\lambda^2(2n_1^2+n_2^2)/(2\alpha)^2} \sum_{j=1}^{N} e^{-i2\pi[n_1(y_j-x_j)+n_2z_j]/a}
$$

Since there is no additional periodic zero in the summation over $(x_j, y_j, z_j)$ in Eq. (25), the expansion in Eq. (24) is the correct Fourier expansion of $V_{2D}(x, y)$ for solving the Bloch eigenstates. As shown in Fig. 2b, there are four potential wells in each unit cell and the lattice potential is highly anisotropic in the transverse plane. The period of $V_{2D}(x, y)$ are $a_x = a/\sqrt{2}$ and $a_y = a$ along the $[\overline{1}10]$ and $[001]$ crystal axes that are the axes of the primitive unit cell in the transverse plane for a beam channeling through a diamond-like crystal along the $[110]$ crystal axis.

c. Channeling along $[111]$ Crystal Axis

For a beam channeling in $[hkl] = [111]$ direction, $\theta_1 = \arctan(k/h) = \pi/4$ and $\theta_2 = \arctan(l/\sqrt{h^2+k^2}) = \arctan(1/\sqrt{2})$ for transformation matrix $R$ in Eq. (8) and $h_y = -hl = -1$, $k_y = -kl = -1$, and $l_y = h^2 + k^2 = 2$ for the Miller indices of one crystal direction for the transverse coordinates. The $x$ and $y$ coordinate are therefore aligned with $[kh0] = [\overline{1}10]$ and $[h_y k_y l_y] = [\overline{1}12]$ crystal axes, respectively. The transformation of the reciprocal lattice vector is calculated from Eq. (10) as

$$
\left( \frac{k_2 - k_1}{\sqrt{2} a} , \frac{k_3 - k_1 - k_2}{\sqrt{6} a} , \frac{k_1 + k_2 + k_3}{\sqrt{3} a} \right) = \left( \frac{n_1}{b_1} , \frac{n_2}{b_2} , \frac{n_3}{b_3} \right)
$$
For integer \((k_1, k_2, k_3)\) and \((n_1, n_2, n_3)\), the solution of Eq. (26) with the minimal values of \((b_1, b_2, b_3)\) at \(n_3 = 0\) is

\[
\begin{align*}
(b_1, b_2, b_3) &= \left(\frac{a}{\sqrt{2}}, \frac{a}{\sqrt{6}}, \sqrt{3}a\right) \\
(k_1, k_2, k_3) &= (-n_1 - n_2, n_1 - n_2, 2n_2)
\end{align*}
\] (27)

The 2D lattice potential can then be calculated from Eqs. (12), (13), and (6) as

\[V_{2D}(x, y) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} V_{n_1n_2} \exp \left[i2\pi \left(\frac{n_1x}{a/\sqrt{2}} + \frac{n_2y}{a/\sqrt{6}}\right)\right] \] (28)

where

\[V_{n_1n_2} = -\frac{2\pi \hbar^2}{m_ee^2} \sum_{i=1}^{M} \frac{\alpha_i}{a} e^{-\lambda_i^2(n_1^2 + 3n_2^2)/2a^2} \sum_{j=1}^{N} e^{i2\pi[n_1(x_j - y_j) + n_2(x_j + y_j - 2z_j)]/a} \] (29)

With the ion coordinates \((x_j, y_j, z_j)\) given in Table I, the second summation in Eq. (29) can be evaluated as

\[\sum_{j=1}^{N} e^{i2\pi[n_1(x_j - y_j) + n_2(x_j + y_j - 2z_j)]/a} = \begin{cases} 8, & \text{for } n_1 + n_2 = \text{even} \\
0, & \text{otherwise} \end{cases} \] (30)

and \(V_{n_1n_2}\) can thus be rewritten as

\[V_{n_1n_2} = -\frac{16\pi \hbar^2}{m_ee^2} \left(\sum_{i=1}^{M} \frac{\alpha_i}{a} e^{-\lambda_i^2(n_1^2 + 3n_2^2)/2a^2}\right) \delta_{n_1+n_2,\text{even}} \] (31)

Because of different periodicity of \(V_{2D}(x, y)\) in Eq. (28) along the \(x\) and \(y\) direction, the periodic occurrence of zero in \(V_{n_1n_2}\) cannot be removed from the summations in Eq. (28) by relabeling the summation indices and a rotation of \((x, y)\) coordinate while keeping the form of a Fourier expansion. This can also be seen in the contour plot of \(V_{2D}(x, y)\) in Fig. 2c, where there are two identical potential wells at the corners and center of a unit cell and it cannot be simplified into a single square lattice because of different lattice constants along the \(x\) and \(y\) direction. The \([\bar{1}0]\) and \([\bar{1}12]\) crystal axes are therefore the orthogonal axes of the primitive unit cell in the transverse plane and \(a_x = a/\sqrt{2}\) and \(a_y = a/\sqrt{6}\) are the correct periods of \(V_{2D}(x, y)\) for a beam channeling in the \([111]\) direction.

d. Channeling along \([210]\) Crystal Axis

For a beam channeling along the \([hkl]\) = \([210]\) crystal axis, \(\theta_1 = \arctan(k/h) = \arctan(1/2)\) and \(\theta_2 = \arctan(l/\sqrt{h^2 + k^2}) = 0\) and the solution of Eq. (10) is

\[
\begin{align*}
(b_1, b_2, b_3) &= \left(\frac{a}{\sqrt{5}}, a, \frac{a}{\sqrt{5}}\right) \\
(k_1, k_2, k_3) &= (-n_1 + 2n_3, 2n_1 + n_3, n_2)
\end{align*}
\] (32)
The lattice potential with \( x \) and \( y \) coordinate aligned with \([\bar{k}hl] = [\bar{1}20]\) and \([h_yk_yl_y] = [001]\) crystal axes can be calculated from Eqs. (12), (13), and (6) as

\[
V_{2D}(x, y) = \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} V_{n_1n_2} \exp \left[ i2\pi \left( \frac{n_1x}{a/\sqrt{5}} + \frac{n_2y}{a} \right) \right]
\]  

(33)

where

\[
V_{n_1n_2} = -\frac{2\pi \hbar^2}{m_e a^2} \sum_{i=1}^{M} \frac{\alpha_i}{a} e^{-\lambda_i^2(5n_1^2+n_2^2)/(2a)^2} \sum_{j=1}^{N} e^{-i2\pi[n_1(2y_j-x_j)+n_2z_j]/a}
\]

(34)

With ion coordinates \( \vec{r}_j \) in a unit cell given in Table I, the summation over the ions in Eq. (34) is

\[
\sum_{j=1}^{N} e^{-i2\pi[n_1(2y_j-x_j)+n_2z_j]/a} = \begin{cases} 
4 \left[ 1 + (-1)^{(n_1+n_2)/2} \right], & \text{for } (n_1, n_2) = (\text{even, even}) \\
0, & \text{otherwise}
\end{cases}
\]

(35)

Similar to the case of the channeling in the [001] direction, this periodic occurrence of zero in the Fourier expansion can be removed by relabelling the summation indices as \( n_1 = 2k_1 \) and \( n_2 = 2k_2 \) in Eq. (33) without altering the form of the Fourier expansion. The periods of \( V_{2D}(x, y) \) in this case is thus \( a_x = a/(2\sqrt{5}) \) and \( a_y = a/2 \) along the \([\bar{1}20]\) and \([001]\) crystal axes, respectively, and the Fourier expansion of the 2D lattice potential in Eq. (33) should be rewritten as

\[
V_{2D}(x, y) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} v_{k_1k_2} \exp \left[ i2\pi \left( \frac{k_1x}{a/(2\sqrt{5})} + \frac{k_2y}{a/2} \right) \right]
\]

(36)

where

\[
v_{k_1k_2} = -\frac{8\pi \hbar^2}{m_e a^2} \sum_{i=1}^{M} \frac{\alpha_i}{a} e^{-\lambda_i^2(5k_1^2+k_2^2)/a^2} \left[ 1 + (-1)^{k_1+k_2} \right]
\]

(37)

where \( v_{k_1k_2} = 0 \) for \( k_1+k_2 = \text{odd} \). As shown in Fig. 2d, there are two identical potential wells in each unit cell of \( V_{2D}(x, y) \). Similar to the case of channeling in the [111] direction, this 2D body-center rectangular unit cell cannot be simplified into a simple rectangular unit cell because of different periodicity of \( V_{2D}(x, y) \) along the \( x \) and \( y \) direction. The \([\bar{1}20]\) and \([001]\) crystal axis are the orthogonal axes of the primitive unit cell in the transverse plane and \( a_x = a/(2\sqrt{5}) \) and \( a_y = a/2 \) are the correct periodicity of \( V_{2D}(x, y) \) for a beam channeling through a diamond-like crystal along the \([210]\) crystal axis.
IV. FINAL REMARKS

To solve the Bloch eigenstates for the transverse motion of beam electrons in a crystal numerically, the Fourier expansion of the lattice potential in Eq. (12) needs to be truncated as

\[ V_{2D}(x, y) = \sum_{n_1=-K_{\text{max}}}^{K_{\text{max}}} \sum_{n_2=-K_{\text{max}}}^{K_{\text{max}}} V_{n_1n_2} e^{i2\pi(n_1x/b_1+n_2y/b_2)} \]  

(38)

This truncation is possible due to a fast decay of expansion coefficient \( V_{n_1n_2} \) which is the consequence of an electron-ion interaction potential that decays faster than \( 1/r \). The convergence of the truncation, however, needs to be checked to ensure the accuracy of the numerically calculated potential. To examine the convergence, we estimate the truncation error using

\[ \text{Truncation Error} = \frac{1}{a_xa_y} \int_0^{a_y} \int_0^{a_x} \left| \frac{V_{2D}(x, y, K_{\text{max}})}{V_{2D}(x, y, K_{\text{max}} + \Delta)} - 1 \right| \, dx \, dy \]  

(39)

where \( V_{2D}(x, y, K_{\text{max}}) \) and \( V_{2D}(x, y, K_{\text{max}} + \Delta) \) are the lattice potential \( V_{2D}(x, y) \) calculated with the truncation at \( K_{\text{max}} \) and \( K_{\text{max}} + \Delta \), respectively. Figure 3 plots this truncation error as a function of \( K_{\text{max}} \) for the examples in Fig. 2 and shows that the numerically calculated potential is sufficiently accurate (with a truncation error smaller than \( 10^{-8} \)) for \( K_{\text{max}} < 50 \). Note that solving the Bloch eigenstates numerically from a two-dimensional Schrödinger equation requires diagonalizations of \( (2K_{\text{max}} + 1)^2 \times (2K_{\text{max}} + 1)^2 \) matrices for the Hamiltonian operator and, with \( K_{\text{max}} < 50 \), this computational task can be handled with well-configured pc computers nowadays.

In summary, we have developed a general formalism for the lattice potential for studying the transverse motion of beam electrons when an ultra-relativistic beam channels through a crystal lattice. As shown by the examples, this two-dimensional lattice potential can easily be calculated for a beam channeling through a crystal along any crystal direction. With the availability of the 2D lattice potential and increasing power of pc computers, the 2D calculation of the Bloch eigenstates should becomes the standard for the study of the channeling radiation and the 1D approximation in modeling the channeling radiation is no
longer needed.

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Table I. Ion position $\vec{r}_j$ in a unit cell of diamond-like crystals where the origin of the coordinate is at a corner of the unit cell and $a$ is the lattice constant.

| $j$ | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  |
|-----|----|----|----|----|----|----|----|----|
| $x_j/a$ | 0  | $1/4$ | 0  | $1/4$ | $1/2$ | $3/4$ | $1/2$ | $3/4$ |
| $y_j/a$ | 0  | $1/4$ | $1/2$ | $3/4$ | 0  | $1/4$ | $1/2$ | $3/4$ |
| $z_j/a$ | 0  | $1/4$ | $1/2$ | $3/4$ | $1/2$ | $3/4$ | 0  | $1/4$ |

Table II. Fitting parameters $\alpha_j$ and $\beta_j$ for atomic form factor of germanium obtained by Chouffani and Überall [18], where $a = 5.658\text{Å}$ is the lattice constant.

| $i$ | 1  | 2  | 3  | 4  | 5  | 6  |
|-----|----|----|----|----|----|----|
| $\alpha_i/a$ | 0.3204585 | 0.4895285 | 0.1625405 | 0.0121414 | 0.0427155 | 0.0027543 |
| $\beta_i/a^2$ | 2.0642597 | 0.6336834 | 0.0351070 | 0.0010696 | 0.0073946 | 0.1409283 |
Figure 1. (a) The \([hkl]\) and \([hk0]\) crystal axis in the lattice coordinate \((X_1, X_2, X_3)\) of an orthorhombic crystal lattice, (b) the 1st coordinate rotation on the \(X_1-X_2\) plane and (c) the 2nd coordinate rotation on the \(X'_1-X_3\) plane for the construction of \(R\) for a beam channeling in \([hkl]\) direction, where \(\theta_1 = \arctan(k/h)\) and \(\theta_2 = \arctan(l/\sqrt{h^2 + k^2})\). The crystal axis \([h_yk_yl_y]\) is along the direction of integer vector \((h_y, k_y, l_y) = (h, k, l) \times (-k, h, 0) = (-hl, -kl, h^2 + k^2)\).
Figure 2. Contour plots of lattice potential $V_{2D}(x, y)$ on the beam transverse plane for a beam channeling through a diamond-like crystal along (a) [001], (b) [110], (c) [111], and (d) [210] direction, where $a_x$ and $a_y$ are the periods of $V_{2D}(x, y)$ in the $x$ and $y$ direction, respectively, and $V_{\text{min}}$ and $V_{\text{max}}$ are the minimum and maximum of $V_{2D}(x, y)$. The centers of equipotential loops are the bottoms of potential wells.
Figure 3. Truncation error of the truncated Fourier expansion of $V_{2D}(x,y)$ in Eq. (38) v.s. $K_{max}$ calculated using Eq. (39) with $\Delta = 5$ for channeling of germanium along the [001] (circles), [110] (squares), [111] (triangles), and [210] (stars) crystal axis, respectively.