Basic Channeling with Mathematica©: a New Computer Code

O V Bogdanov, E I Fiks, K B Korotchenko, Yu L Pivovarov, T A Tukhfatullin
Tomsk Polytechnic University, Tomsk, 634050 Russia
korotchenko@tpu.ru

Abstract. The Mathematica© software is a powerful tool to solve numerous problems in physics, essentially when the analytical solution is not possible. The channeling and related phenomena is just that case. Here we suggest to introduce a “standard” in calculations of channeling and related phenomena using Mathematica© software. The new computer code “Basic Channeling with Mathematica©” BCM–1.0, at the first stage, will include a set of packages to make symbolic calculation of the planar channeling phenomena.

1. Introduction
The analysis of channelling and related phenomena (e.g. channelling radiation, diffracted channelling radiation, etc.) is connected with cumbersome analytical and numerical calculations. The new computer code BCM 1.0 is created to avoid these difficulties and introduce “the standard” in these calculations. The “standard” problems in planar channeling are:

- calculation of planar periodic potential function \( U(r_x) \) for chosen set of crystallographic planes of desired crystal;
- computation of classical trajectories of channeled charged particles in defined periodic potential function \( U(r_x) \);
- computation of eigenvectors (i.e. wave functions) and eigenvalues (i.e. energy levels) of channeled electrons (positrons) transverse motion in defined periodic potential function \( U(r_x) \);
- calculation of transverse energy levels initial populations;
- calculation of transitions matrix elements of channeled electrons (positrons).

Our solution experience of these problems using Mathematica© software has allowed us to attack the problem of creation the library of packages for the radiation problems at the channeling solution – “Basic Channeling with Mathematica©”(BCM).

The first version of the new computer code – BCM 1.0 includes the following packages:

- “Potential.m” – computation of continuous potential function of the crystallographic planes \( U(y) \).
- “Trajectory.m” – computation of classical channeled charged particles trajectories in planar periodic potential function \( U(y) \).
- “Eigen.m” – solution of eigenvalue problem to determine transverse energy band structure and eigenfunctions from the Schrödinger equation with relativistic mass of channeled electron (positron) in periodic potential function \( U(y) \).
• “Population.m” – computation of initial populations of transverse energy bands using “Eigen.m”.
• “Matrix.m” – computation of transitions matrix elements (in dipole approximation) using “Eigen.m”.

2. Planar channeling potential function
Good description for planar potential function \( U(y) \) of real crystal one can obtain from formula given by Doyle and Turner [1] for single atom potential function by fitting the electron scattering form factor with experimental parameters \( a_j \) and \( b_j \):

\[
U_{at}(\vec{r}) = -(2h^2 / \sqrt{\pi m_e}) \sum_j a_j c_j^{-3/2} \exp(-r^2 / c_j^2).
\]  

(1)

Here, \( 4\pi^2 c_j = b_j + 8\pi^2 \rho_j^2 \) and \( \rho_j \) is the amplitude of thermal vibrations of atom. Integration of the formula (9) along channeling plane \( (XZ-\text{plane}) \) leads to separate plane potential function

\[
U_{pl}(y) = -A \sum_j a_j c_j^{-3/2} \exp(-y^2 / c_j^2),
\]

(2)

where \( A = 16\sqrt{\pi r_c} \rho_c \), \( r_c = 27.2116d / a \), \( d \) is the interplanar spacing, \( a \) is a lattice constant, \( r_c \) is the Bohr radius.

In the case of complex crystal, the periodic potential function \( U(y) \) is obtained by summation of potential functions \( U_{pl}(y) \) over the single planes for all kinds of atoms in crystal. For example, total planar potential function for (111) LiF is

\[
U(y) = \sum_m (U_F(y + md) + U_L(y + md - d / 2)),
\]

(3)

where \( m \) is the minimal number of single planes for the necessary precision of the total planar potential function \( U(y) \) computation.

Next we may calculate Fourier components of the potential function \( U(y) \)

\[
U_m = \int_{d/2}^{d/2} U(y) \exp(-im \cdot g \cdot y) dy,
\]

(4)

3. Classical trajectory of planar channelled charged particles in crystals
The motion equation for the classical relativistic charged particle in the field with potential function \( U(y) \) for the transverse direction (in the approximation of \( \nu_\perp \equiv \dot{y} \ll \nu_\parallel; \nu_\perp / c \ll 1 / \gamma \) ) has the form (see in Fig.1)

\[
\gamma m \ddot{y} = -\frac{\partial U(y)}{\partial y}, \quad \gamma = \frac{1}{\sqrt{1 - v_\perp^2 / c^2}}
\]

(5)

where \( \nu_\parallel \) is the average electron’s velocity along the channel and \( \nu_\perp \) is the velocity of transverse motion. The initial conditions are: the point of incidence into a crystal \( y(0) = y_0 \) and transverse momentum \( p_\perp(0) = p_\parallel \sin \theta_0 \cong p_\parallel \theta_0 \), where \( p_\parallel = m \nu_\parallel \) and \( \theta_0 \) is the electron incidence angle with respect to the channeling plane. They determine the integral of motion equation, the so-called transverse energy:

\[
e_\perp = U(y) + \frac{p_\perp^2}{2 \gamma m} = U(y_0) + \frac{p_\parallel^2 \theta_0^2}{2 \gamma m}.
\]

(6)
4. Eigensystem problem: a theoretical background

The wave function $\Psi(r,t)$ of the planar channeled electron with an energy $E > 1$ MeV may be written as $[2]$

$$\Psi(r,t) = \exp(-i(p_z - Et)/\hbar)\phi(y).$$  \hspace{1cm} (7)

Here, $Y$–axis is perpendicular to the channeling plane, $p_\parallel$ is the longitudinal momentum (along the channeling plane and $Z$–axis – see Fig.1). The wave function (7) is the solution of the Klein–Gordon equation with potential function $U(y)$, which transforms into Schrödinger equation with relativistic mass $\gamma m_e$ when $2E_\parallel >> (E_\perp - U(y))$ $[2]$

$$2m_\gamma(E_\perp - U(y))\phi(y) = -\hbar^2 \partial^2_y \phi(y).$$  \hspace{1cm} (8)

Here, $\gamma$ is relativistic factor, $E_\parallel = \sqrt{(cp)^2 + m_e^2 c^4}$ and $E_\perp$ is the energy of electron transverse motion. In the periodic potential function $U(y)$ wave function $\phi(y)$ and energy of transverse motion of electron $E_\perp$ are continuous functions of $Y$–component electron wave vector $k_y$, which lies in the first Brillouin zone (e.g., see$[3]$). Therefore, $\phi(y) \rightarrow \phi(y,k_y)$, $E_\perp \rightarrow E^\parallel_\perp(k_y)$.

The standard method of solving the Schrödinger equation (5) in accordance with the Bloch form of wave function of electron $\phi^i(y,k_y)$ in the periodic potential function $U(y)$ consists in use of the Fourier expansion of wave function $\phi^i(y,k_y)$

$$\phi^i(y,k_y) = \sum_m C^i_m(k_y)\exp\{i(k_y + m|g|)y\}/d,$$  \hspace{1cm} (9)

and potential function $U(y)$

$$U(y) = \sum_m U_m \exp\{im|g|y\},$$  \hspace{1cm} (10)

Here, $g$ is the reciprocal lattice vector of channeling planes, $U_m$ are the Fourier components of potential function $U(y)$. Then we substitute equations (9) and (10) into (8) and obtain eigensystem problem $[1], [4–5]$:

$$\sum_m A_{mn} C^i_m(k_y) = E^\parallel_\perp(k_y)C^i_0(k_y), \hspace{0.5cm} A_{mn} = U_{m-n} + \delta(m,n)(\hbar^2(m|g|+k_y)^2/2m_\gamma),$$  \hspace{1cm} (11)
where $\delta(m,n)$ is the Kronecker delta.

5. Calculation of planar channeling potential function

With new computer code BCM 1.0 calculation of planar channeling potential function $U(y)$ and its Fourier components $U_m$ starts with work directory setting and package “Potential.m” attaching (see Fig.2).

```
SetDirectory["C:\Electron\Potential\"];
Print << BCM\Potentials.m;
Si[[1, 1, 1]];
PotentialU[7];
```

```
0.4\[y\]^2
Potential U[\[y\]], eV

Potential U[\[y\]], eV

0.4\[y\]^2
```

**Figure 2.** Computation example with package “Potential.m”.

The package “Potential.m” consist of following subroutines:

- **ElementName[[Plane]]** – to choice a crystal (now only Si, LiF and Ge are available) and plane (in form of Miller indices). For example: Si[[1,1,1]] – Fig2.
• **PotentialU[Np]** – computation of the periodic planar potential function \( U(y) \) (in eV of Å) for the selected crystallographic plane (i.e. (111) Si for above mentioned example). Here, \( Np = 2m + 1 \) (\( m \) from Eq. (11)) is the minimal number of single planes for the necessary precision of the total planar potential function \( U(y) \) computation. For example: PotentialU[7] – Fig2.

• **GraphU[Np]** – to display the plot of function \( U(y) \). For example: GraphU[7] – Fig2.

• **FourierImageU[Np]** – computation of the Fourier components \( U(m) \) of the planar potential function \( U(y) \) using formula (5). For example: FourierImageU[7] – Fig2.

• **GraphFU[NN]** – to display the plot of function \( U(y) \) calculated by his Fourier components \( U(m) \). Here, \( NN \) is number of Fourier components for the plot of the planar potential function \( U(y) \). For example: GraphFU[13] – Fig2.

The functions PotentialU[Np] and FourierImageU[Np] save the results of calculation potential function \( U(y) \) and its Fourier components \( U(m) \) in special folder with name forming by crystallographic plane. For the selected plane, i.e. (111) Si (for above mentioned example) “Data-Si-111” into directory specified by you – “C:/Electron/Potential” (see in Fig2).

6. **Calculation of classical trajectory**

To solve the differential equation (5) with the help of the software suite Mathematica© we have developed sufficiently simple and high–performance algorithm [7–8].

For solution differential equation (5) using BCM 1.0 the package “Trajectory.m” is used. This package consists of subroutines:

• **ElementParticle[{Plane, m, q}]** – to choice the particle parameters: mass \( m \) (in MeV) and charge \( q \) (in chadage of electron); and the crystal (now only Si, LiF and Ge are available) and plane (in form of Miller indices). For example: ElementParticle[Si[{1,0,0}, 0.511, 1].

• **Period[Xo, Θo, Eo]** – computation the period (in sec.) of transverse motion of charged particle with initial parameters: coordinate \( Xo \) (in \( d \), i.e. in the interplanar spacing), initial angle with respect to the channeling planes \( Θo \) (in Lindhard critical angle \( Θθ_c \)) and energy \( Eo \) (in MeV).

For example: Period [0.25, 0.2, 1000] equal 8.30866×10^{-15} sec. (for above mentioned example).

• **FourierImagePath[Xo, Θo, Eo]** – computation of the Fourier components of \( y = y(t) \) is classical trajectory of planar channelled charged particle in crystal with initial parameters \( Xo, Θo, Eo \).

• **GraphPath[Xo, Θo, Eo]** – to display the trajectory plot \( y = y(t) \) of channelled particle with initial parameters: \( Xo, Θo \) and \( Eo \).

This package uses the period planar potential function \( U(y) \) calculated by “Potentials.m”.

7. **Solution of eigensystem problem**

The experience of solving the problem (11) with the help of the software suite Mathematica© allowed us develop sufficiently simple and high–performance algorithm [7–8].

For solution of eigensystem problem (11) in BCM 1.0 there is the package “Eigen.m”:

• **EigenSystem[“Name”, {Plane}, NN, Np]** – computation the Fourier components \( C_m^i(k_y) \) of the wave functions \( φ_i(y,k_y) \) for \( i^{th} \) quantum state and eigenvalues, i.e. energies \( E_i^⊥(k_y) \) (in eV) of channeled electrons occupying these \( i^{th} \) quantum state. Here, \( NN \) is the number of Fourier components \( C_m^i(k_y) \) and \( Np \) is the minimal number of single planes for the necessary precision of the total planar potential function \( U(y) \) computation.
For example: EigenSystem[“Si”, {111}, 20, 7] – Fig.3.

This package uses the Fourier component $U(m)$ of planar potential function $U(y)$ calculated earlier with “Potentials.m”. This package saves the results of calculation: Fourier components $C_n(k_y)$, energies $E_y^+(k_y)$ and matrix $A_{mn}$ from Eq.(11) in special folder with name “alm” into directory specified by you. For example in Fig2. – “C:\Electron\Potential\Data-Si-111\”.

8. Calculation of dipole transition matrix elements: package “Matrix.m”

The planar channeling of relativistic particles is accompanied by spontaneous radiation due to transitions between the energy levels $E_y^+(k_y)$ and $E_y^+(k_y)$ of the transverse motion. For calculation of channeling radiation probability in dipole approximation, the transition matrix elements are required

$$\gamma_y(k_y^i,k_y^f) = \langle \phi^+(y,k_y^i) | \phi^-(y,k_y^f) \rangle.$$

In packages of BCM-01, by performing calculations of initial population and transition matrix elements, we divide the first Brillouin zone into $N = 10$ equal parts.

Then we denote $\gamma_y(k_y^i,k_y^f)$ $\gamma[i, ni, f, nf]$ where $i$ and $f$ are the quantum state numbers of electron transverse motion at planar channeling, $ni$ and $nf$ are the numbers of $n^{th}$ part of the $i^{th}$ and $f^{th}$ quantum states.

By performing calculation using the package “Matrix.m”:

- MatrixElement[Name, gamma] – to calculate matrix elements $\gamma[i, ni, f, nf]$ in dipole approximation for electrons with $\gamma = gamma$ channeled along the crystallographic planes Name, and for transition between the quantum states $i_{ni} \rightarrow f_{nf}$.

For example: MatrixElement[(111)LiF, 20] – calculation of dipole transition matrix element at planar channeling electron with $\gamma = 20$ along (111)LiF. Then, $\gamma[0, 5, 3, 10]$ is the matrix element for transition $3_{10} \rightarrow 0_5$ at planar channeling electron with $\gamma = 20$ for (111)LiF.

9. Calculation of transverse quantum states initial populations: package “Population.m”

For calculation of channeling radiation from relativistic electron beam entering a crystal, it is necessary to know initial populations of transverse energy levels. It is the probability that a free electron entering at a small angle with respect to the crystallographic planes may be captured to one of the possible transverse energy levels

$$P_y(k_y^i,k_y^f) = \left| \left\langle \phi^+(y,k_y^i) | \phi^-(y,k_y^f) \right\rangle \right|^2 / d,$$

where $\phi^+(y,k_y^i) = \exp(-i k_y^i y)$ is the wave function for transverse motion of incident free electron with wave vector $k = (k_x,k_y)$, . The wave vector $k$ components of free electron are defined as: $k_y = p_y / h$, $k_x = p_x(0) / h \equiv p_x \theta_x / h$.
In the package “Population.m” we denote \( P_i(k_x, k_y) \rightarrow pP[i, ni, nk] \), where \( i \) is the quantum state numbers of electron transverse motion at planar channeling, \( ni \) is the number of \( n^\text{th} \) part of the \( i^\text{th} \) quantum state and \( nk \) is the number of \( n^\text{th} \) part of the \( \theta_L \) – Lindhard critical channeling angle.

We divide the Lindhard critical angle \( \theta_L \) into \( N_L = 15 \) equal parts. The package calculate initial populations till \( nk = 30 \), that is till initial angle \( \theta_0 = 2\theta_L \).

By performing calculation using the package “Population.m”:

- **InitialPopulation[Name, gamma]** – to calculate initial populations \( pP[i, ni, nk] \) of quantum states (with numbers \( i, ni, nk \)) by free electrons with \( \gamma = gamma \) entering a crystal at angle \( \theta_o = \theta_L nk / 30 \) with respect to the channeling planes \( Name \).

For example: InitialPopulation[(111)LiF, 20] – calculation of initial population at planar channeling of electrons with \( \gamma = 20 \) along (111)LiF. Then, \( pP[3, 10, 5] \) is initial population of quantum state \( 3 \) by free electrons entering a crystal at angle \( \theta_0 = 5\theta_L / 30 \) with respect to the channeling planes (111)LiF.

10. **Comments for users**

The packages “Matrix.m” and “Population.m” use the matrix \( A_{mn} \) calculated earlier with package “Eigen.m”.

Before using the packages “Potentials.m”, “Trajectory.m”, “Eigen.m”, “Matrix.m” and “Population.m” one must put these packages in special folder of Mathematica® which is reserved for external packages. For example, put all packages in folder “BCM” and put this folder in directory “C:\Program Files\Wolfram Research\Mathematica\6.0\AddOns\Packages”. Then you can use computer code BCM 1.0 as in Figs.2,3.

11. **Conclusions**

The 1st version of new computer code BCM–1.0 is presented. To start calculations, one needs the Mathematica® 6.0 version, necessary packages from [9] and standard personal computer (e.g. Intel(R) Core(TM)2 CPU 2 GHz, 2 Gb of RAM).

The beta–version of BCM–1.0 is available for testing [9].

The future developments will include:

- Calculation of planar CR spectra (classical).
- Calculation of planar CR spectra (quantum).
- Calculation planar DCR and PXRC.
- Calculation of axial CR spectra (classical).
- Calculation of axial CR spectra (quantum).
- Calculation of axial DCR.

Then we plan to include inelastic processes, e.g. multiple scattering, energy loss, dechanneling etc.

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