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BCM-2.0 – The new version of computer code "Basic Channeling with Mathematica©"

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ABSTRACT

The new symbolic-numerical code devoted to investigation of the channeling phenomena in periodic potential of a crystal has been developed. The code has been written in Wolfram Language taking advantage of analytical programming method. Newly developed different packages were successfully applied to simulate scattering, radiation, electron-positron pair production and other effects connected with channeling of relativistic particles in aligned crystal. The result of the simulation has been validated against data from channeling experiments carried out at SAGA LS.

1. Introduction

When relativistic charge particles are incident on a single crystal, several phenomena can occur, reflecting the periodic arrangement of atoms in the crystal. If particles are injected into a crystal almost parallel to a crystallographic axis or plane, they become trapped by the associated potential and their motion is guided by it; this process is referred to as channeling.

Several software packages based on various model approaches have been developed recently for numerical simulations of the channeling process in straight and bent crystals [1–8]. Most codes are based on the concept of the continuous potential while others use the scheme of binary collisions. "Basic Channeling with Mathematica©" BCM-1.0 is the computer code developed by the authors for simulating channeling related processes [9]. Our code uses the continuous potential model.

The code has been written in Wolfram Language taking advantage of analytical programming method. Wolfram Mathematica has a lot of built-in numerical and analytical functions, visualization and data analysis features, capability of parallel computation using modern multicore CPU and simplicity to include the other programs.

The first version of the computer code allowed to calculate: the planar channeling potential function using Doyle and Turner formula [10] and its Fourier components – package **"Potential.m"**; the classical trajectories of planar channeled charged particles in crystals – package **"Trajectory.m"**; the wave functions of the planar channeled particles – package **"Eigen.m"**; the transverse quantum states initial populations – package **"Populations.m"**.

Newly developed packages were successfully applied to the following problems:

- flux dynamics and angular distributions of relativistic electrons and positrons passing through the thin and half-wave crystals, including mirroring;
- depth oscillations of electronuclear reactions caused by relativistic planar channeled electrons: quantum versus classical calculation;
- optical radiation from channeled relativistic heavy ions in vicinity of the Cherenkov angle;
- angular distribution features of Channeling radiation in the optical range;
- PXRC (parametric X-Radiation at channeling) and its quantum features;

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Table 1
Flux dynamics and particle distribution packages.

Main Package	Functions	Parameters	Goal
Trajectory.m	**Trajx**	*nn* – the total number of calculated trajectories *nθ* – the number of incidence angle for each entry points θ_0 – the incidence angle $\Delta\theta$ – the angular spread of the incidence beam *e0* – initial particle energy in MeV *L*– the crystal thickness in μm	Calculation of *nn* trajectories of channeled particles
	Koordkr3d	*nn* – the total number of calculated trajectories *nt* – the number of points in crystal where the distribution function was calculated *hk* – the transverse coordinate step size	Calculation of the particle distribution function inside the crystal using particle trajectories
Distribution.m	**Koord2d**	*np* – the total number of particles *hm* – the coordinate step size	Calculation of two dimensional beam profiles using initial beam profile shape, exit coordinates and exit angles of particles from a crystal
	Angle2d	*np* – the total number of particles *hθ* – the angle step size	Calculation of two dimensional angular beam distribution using initial beam profile shape, exit coordinates and exit angles of particles from a crystal

Computation time was approximately 25 ms per particle for 255 MeV electrons channeled in 2 μm thick (220) Si crystal.

- radiation energy loss of channeled relativistic electrons in a crystal;
- channeling radiation from electrons in a half-wave crystal;
- positron source via electron-positron pair production by channeling radiation.

Some of these packages have already been used for the simulation of channeling experiment performed at the linac of the SAGA Light Source (SAGA-LS, Japan) [11–13]. The obtained simulation results were in good agreement with the experimental data. Here we want to present the brief description of the new packages and short explanation of the problems that they solve.

In calculations following main approximations were used. The crystal thickness is less than the dechanneling length for a given energy of channeled particles (the dechanneling length value can be obtained in the frame proposed by Baier et al. [14]) – i.e. calculations can be performed only in the case of the "thin crystals". However, crystal should be thick enough to use continuous potential approximation. For example, for 255 MeV electrons channeled in (220) Si, the thickness of the crystal should be more than 0.6 μm and less than 20 μm. The angle of multiple scattering is less than the critical channeling angle for a given energy of channeled particles, so the effect of multiple scattering can be neglected. For 255 MeV electrons channeled in (220) Si the angle of multiple scattering less than critical channeling for crystal thickness equals 10 μm.

The choice of the calculation method depends on the particles energy. For the low energy particles channeled in crystal the quantum description is valid. The minimal energy of channeled particle should be chosen high enough to use continuous potential approximation (approximately 10 MeV for electrons channeled in Si) [15]. The number of quantum energy levels of a particle transverse motion increase with rising of the particle energy When this number is high enough (about 50) the classical approach become valid. For the electrons channeled in Si this condition becomes satisfied at energy $100 \div 150$ MeV. Quantum approach is still valid, but requires more computer resources than the classical one. For the multi-GeV particles the effects of QED become strong and one need to use QED description or quasi-classical approach suggested in [14]. For example, upper border for the applying of classical approach for the description of electrons channeled in Si is 5 GeV.

The tested estimations of computation time were made for computer with 8 GB of RAM and an Intel(R) Core(TM) i7-2600 K CPU 3.40 GHz.

2. Flux dynamics and angular distributions of relativistic electrons and positrons passing through the thin crystals

To obtain the spatial and angular distributions of electrons and positrons at planar channeling one has to calculate the large number of trajectories. Every individual trajectory is calculated by solving classical equations of motion with relativistic mass. For this purpose we use the package from the first version of the computer code BCM-1.0. For each entry point of a particle into a crystal, several values of the incident angle θ are generated randomly with a normal distribution with a certain standard deviation $\Delta\theta$ (Table 1).

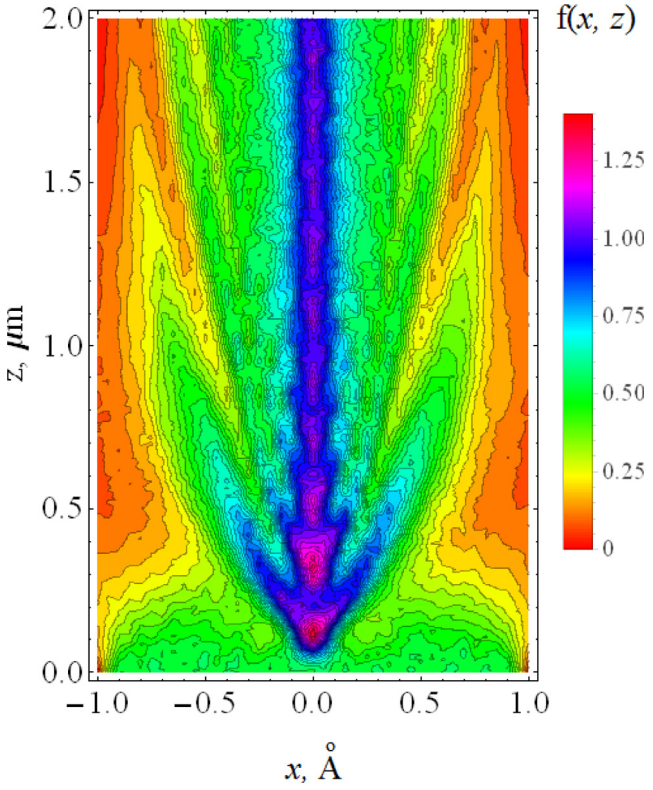

Fig. 1. Spatial distribution of the 255 MeV electrons channeled in 2 μm thick (220) Si crystal. The incident angle of the elections with respect to the channeling plane is $\theta_0 = 0°$, angular spread of the beam is $\Delta\theta = 0.1$ mrad. Entry points were uniformly distributed inside one period of crystal potential (one potential well).

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For example, in the Fig. 1 the result of calculation of the spatial distribution $f(x,z)$ of elections using function **Koordkr3d** is presented. Calculation was performed for 255 MeV electrons channeled in 2 μm thick (220) Si crystal. The incident angle of the elections with respect to the channeling plane is $\theta_0 = 0^o$, angular spread of the beam $\Delta\theta = 0.1$ mrad. Entry points were uniformly distributed inside one period of crystal potential (one potential well). The specific shape of spatial distribution $f(x,z)$ was determined by the form of electron trajectories and electric field which guided the electron motion.

3. Channeling radiation from electrons in a half-wave crystal

The next new package is developed for numerical investigation of the spectral-angular characteristics of the radiation from channeled electrons in a Half-Wave Crystal (HWC). Using the package **"Trajectory.m"** one obtains trajectories of channeled electrons in a HWC and then uses them in calculations based on the formulae of classical electrodynamics [16], which were modified for the case of channeling in a HWC [13]. It should be noted that the radiation spectra are calculated taking into account the characteristics of the initial beam of relativistic electrons: the initial energy, angle of incidence, and the initial angular spread (Table 2).

4. Optical radiation from channeled relativistic heavy ions in vicinity of the Cherenkov angle

This package allows calculating optical radiation from channeled relativistic heavy ions (RHI) in vicinity of the Cherenkov angle. Below only structure and usage of the package are considered, in more detail the influence of planar channeling regime on spectral, angular and azimuthal distributions of optical radiation from RHI was investigated in [17] (Table 3).

5. PXRC (parametric X-radiation at channeling)

Calculations are based on the formula for the angular distribution of PXRC emitted by the channeled electron captured in the n-th quantum state [18]. In our calculation, we summed up over all populated quantum states:

$$\frac{d^3N_{\mathrm{PXRC}}}{d\theta_x d\theta_y dz} = dN_{\mathrm{PXR}} \sum_n P_n(\theta_\circ)|F_{nn}|^2. \tag{1}$$

where dN_{PXR} is an ordinary PXR angular distribution taken in the two-wave approximation, $P_n(\theta_\circ)$ is initial population of n-th energy band and the transverse form factor F_{nn} (Table 4).

6. Depth oscillations of electronuclear reaction yield initiated by relativistic planar channeled electrons: quantum versus classical calculations

The electronuclear reaction can occur in the crystal when channeled relativistic electron moves close to the nucleus, which is in a channeling plane.

In quantum case [20], the convolution of the distribution function $F(x)$ with the flux density $|\Psi(x,z)|^2$ of the planar channeled relativistic electrons should be proportional to the electronuclear reaction yield $Y(z)$, analogously to axial case [21]:

$$Y(z) \sim \int_{-d/2}^{d/2} F(x,z)|\Psi(x,z)|^2 dx,$$

$$F(x,z) = \sum_{i=0}^{N} \frac{1}{2\pi\sigma^2} \exp\left(-\frac{x^2+(z-ai)^2}{2\sigma^2}\right), \Psi(x,z)$$
$$= \sum_n P_n(\theta_0) \exp\left(\mathbf{i}\frac{\varepsilon_n}{\hbar}\frac{z}{c}\right)\varphi_n(x), \tag{2}$$

Table 2
Channeling radiation from electrons packages (classical approach).

Main package	Functions	Parameters	Goal
Spectr.m	**Trajx**	See Section 2	Calculation of *nn* trajectories of channeled particles
SpectrN.m	**FourierField**	θL – the theta-component of radiation angle, φL – the theta-component of radiation angle	Calculation of the Fourier component of the field of channeling of the charged particle in crystal.
	AverageSN	*nn* – the total number of calculated trajectories	Calculation of the radiation spectrum averaged over *nn* trajectories
GraphS.m	To display the radiation spectrum averaged over *nn* trajectories.		

Computation time for **AverageSN** function was approximately 30 s per particle for 255 MeV electron channeled in 2 μm thick (220) Si crystal.

Table 3
Optical radiation from channeled relativistic heavy ions packages.

Main package	Functions	Parameters	Goal
Cherenkov.m	**TrajIon**	*ion_* – RHI – should be defined as {"Au", 197} *x0* – point of incidence θ_0 – angle of incidence *e0* – initial particle energy in MeV/u *L* - radiator thickness in μm	Calculation of both transverse $x(t)$ and longitudinal $z(t)$ RHI trajectories for the planar channeling case; returns 2 arrays: *trajz[t_]* and *trajx[t_]* that contain the values of $z(t)$ and $x(t)$ respectively
	CalcCherenkovRad	*ion_* – RHI – should be defined as {"Au", 197} *radiator* – radiator e.g. "diamond"; λ – radiation wave length in nm; θ – radiation angle; φ – azimuthal angle; *ch* – flag which is used to set the calculation regime: perform calculations in the case of channeling (*ch = 1*) or not (*ch = 0*), for the non-channeling case the transverse coordinate $x(t) = 0$	Calculation of the spectral, angular and azimuthal distributions of the optical radiation in vicinity of the Cherenkov angle in an optically transparent radiator with and without taking into account the planar channeling The function **CalcCherenkovRad** uses the function **TrajIon** to calculate RHI trajectories

Computation time for **CalcCherenkovRad** was approximately 1 min per particle for 2 GeV/u Au ions channeled in 10 μm thick (110) C crystal.

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Table 4
Parametric X-radiation at channeling packages.

Main Package	Functions	Parameters	Goal
FormFactor.m	**WaveFunction**	C_n – Fourier component for n^{th} quantum state n – quantum state number *NN* – Fourier components maximal number	Calculation of transverse wave functions by their Fourier components (calculated with **Eigen.m** [9])
	ValueFF	n – quantum state number θ_o – entering angle d – interplanar space θ_B – Bragg angle	Calculation of transverse form factor F_{nn}
GraphWF.m	Displaying the plot of transverse wave functions for any quantum state (see Ref. [11])		
PXRC.m	**OrdinaryPXR**	d – interplanar space θ_B – Braggs angle χ_0, χ_g – Fourier component of the electric susceptibility (calculated by [19] for the relevant frequencies) θ_x, θ_y – angular coordinates of PXR	Calculation of PXR angular distribution by the dynamic theory formulae [18]
	MaxPXR	d, θ_B, χ_0, χ_g, θ_x and θ_{max} – angular coordinate of PXR maximal intensity	Calculation θ_y^{max} of PXR maximal intensity using the "Mathematica" subroutine "Solve"
GraphPXRC.m	Displaying the plot of PXRC maximal intensity (see Ref. [11])		

Computation time was approximately 3 h for 255 MeV electrons channeled in (220) Si crystal.

where d – is the distance between the channeling planes, x – is the transverse coordinate, z – is the longitudinal coordinate (penetration depth), σ - is the standard deviation, a – is the lattice constant, N – is the number of nuclei along the direction of motion of the electrons, $|\Psi(x,z)|^2$ – is the flux density designed according to Ref. [22], $P_n(\theta_0)$ – is the initial population, n – is the quantum state number, θ_0 – is the angle of incidence of electrons with respect to the channeling planes, ε_n – is the energy of the n-th quantum state, $\varphi_n(x)$ – is the electron transverse wave function of the n-th quantum state (Table 5).

In classical case [22] it is necessary to convolute the probability density $f(x,z)$ with the distribution function $F(x)$ to calculate the electronuclear reaction yield $Y(z)$:

$$Y(z) \sim \int_{-d/2}^{d/2} F(x,z) f(x,z) dx. \quad (3)$$

In both cases (quantum and classical) there are depth oscillations of electronuclear reaction yield $Y(z)$ [20] (Table 6).

7. Total yield of the channeling radiation from relativistic electrons and positrons in the crystals

The total yield of the channeling radiation (CR) from relativistic electrons and positrons can be calculated using the classical expression for the total radiation energy loss of relativistic charged particle moving in electromagnetic field in terms of the trajectory and velocity (or in terms of the fields if **H** = 0) (see, e.g. [16]):

$$\Delta E = \frac{2e^4}{3m^2c^3} \int_0^T dt \frac{\mathbf{E}^2 - (\mathbf{E}\cdot\beta)^2}{(1-\beta^2)}. \quad (4)$$

Here $\boldsymbol{\beta} = \mathbf{v}/c$, $T = L/\upsilon_{||} \approx L/c$ – is the penetration time through a crystal with thickness L, c – is the speed of light, $\upsilon_{||}$ – is the longitudinal velocity of a particle. $\mathbf{E} = -\nabla U(\mathbf{r}_\perp)/e$ – is the transverse electric field of crystal axes or planes, responsible for particle channeling, at any point of calculated trajectory at the moment of time t, m and e - are the particle mass and charge, respectively (Table 7).

Table 5
Depth oscillations of electronuclear reaction yield packages (quantum approach).

Main package	Functions	Parameters	Goal
ERQ.m	**WaveFunction**	C_n – Fourier component for n^{th} quantum state n – quantum state number *NN* – maximal number of Fourier components	Calculation of the transverse wave functions of the planar channeling electron by their Fourier components (calculated with **Eigen.m** [9])
	QuantumFlux	θ_0 – the angle of incidence of electrons with respect to the channeling planes	Calculation of the flux density of the channeled relativistic electrons determined by the transverse wave function and initial population (calculated with **Population.m** [9])
	ERQ	Θ_D – Debye temperature T – temperature of crystal	Calculation of the electronuclear reaction yield initiated by relativistic planar channeled electrons (quantum calculations)

Computation time was approximately 4.5 h for 255 MeV electrons channeled in (220) Si crystal.

Table 6
Depth oscillations of electronuclear reaction yield packages (classical approach).

Main package	Functions	Parameters	Goal
ERC.m	**ClassicalFlux**	*nn* – total number of calculated trajectories *nt* – number of points in crystal where the distribution function was calculated *hk* – the transverse coordinate step size	Calculation of the flux density of channeled electrons inside the crystal
	ERC	Θ_D - Debye temperature T – temperature of crystal	Calculation of the electronuclear reaction yield initiated by relativistic planar channeled electrons (classical calculations)

Computation time (see, in Section 2.).

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Table 7
Total yield of the channeling radiation packages.

Main package	Functions	Parameters	Goal
TotalCRyield.m	**EPCRyield**	See parameters of **Trajectory.m.**	Calculation of the total yield of CR from electrons or positrons at axial or planar channeling (using **Trajectory.m** [14] which determines beam energy, particle, crystal and channeling type and entering angle)
	AlDCRyield	$\Delta\theta$ – the angular spread of the incidence beam	Calculation of the angular-of-incidence dependence of total yield of CR from electrons or positrons at axial or planar channeling (uses **EPCRyield** function)

Computation time was approximately 3 s per particle for 255 MeV electrons channeled in 2 μm thick (220) Si crystal.

Table 8
Positron source via e- e + pair production by channeling radiation packages.

Main package	Functions	Parameters	Goal
PosSource.m	**PosBarn**	$W(\omega)$ – intensity spectrum of the radiation used for positron production Z – atomic mass of converter E_γ is the energy of the photon E_p is the total energy of positron	Calculation of the e^-–e^+ pair production cross-section by CR (6) using **SpectrN** (Section 4)
	PosSpect	*See* **PosBarn**	Calculation of the energy spectrum of positrons from conversion of CR into e^-–e^+ pair (uses **PosBarn** function)
	PosYield	*See* **PosBarn**	Calculation of the total yield of positrons from conversion of CR into e^-–e^+ pair (uses **PosSpect** function)

Computation time for was approximately 45 minutes using previously saved $W(\omega)$.

Using the package **"TotalCRyield.m"**, the angle-of-incidence dependence of the total yield of channeling radiation in a thin crystal has been studied [23]. Angle-of-incidence dependence of the total yield of the CR can be used for the thin crystal alignment in more complicated channeling experiments and, even more, for diagnostics of angular spread of moderately relativistic electron or positron beams.

8. Positron source via e^- e^+ pair production by channeling radiation

Also in this version of computer code we developed several packages for evaluation of energy spectra of positrons which can be produced in the two-component (hybrid) scheme. The electron beam enters into a crystalline target (radiator) to produce channeling radiation (CR), emitted photon beam is separated from charged particles and directed onto amorphous target (convertor) for conversion into e^-–e^+ pairs.

The cross-section of e^-–e^+ pair production by CR:

$$\frac{d\sigma_{CH}(Z,E_P,E_\gamma)}{dE_P} = \frac{1}{E_\gamma}\frac{dW}{dE_\gamma}\cdot\frac{d\sigma(Z,E_P,E_\gamma)}{dE_P}, \quad (5)$$

here E_γ – is the energy of the photon and E_p – is the total energy of positron, Z – is the atomic number of the converter material, $d\sigma(Z,E_P,E_\gamma)/dE_P$ – is the Bethe-Heitler cross-section of e^-–e^+ pair production by photon in atomic field [24], dW/dE_γ – is the CR intensity that is calculated using the function ***SpectrN*** described in Section 3.

In the frame of considered hybrid scheme, the yield of positrons from conversion of CR into e^-–e^+ pair per convertor of thickness L_c is determined by the expression:

$$Y_P = n\cdot L_C\cdot\iint\frac{d\sigma_{CH}(Z,E_P,E_\gamma)}{dE_P}dE_\gamma dE_P \quad (6)$$

where n is the number of atoms per volume unit of converter, L_C – is the convertor thickness (Table 8).

The new package allows calculation of energy spectra and total yield of the positrons in the frame of the hybrid scheme of positron source using CR from 100 to 1600 MeV electrons and thin amorphous converter [25].

9. Conclusions

The new version of computer code "Basic Channeling with Mathematica©" BCM-2.0 is presented. New developed packages of this code were successfully applied to the following problems: flux dynamics and angular distributions of relativistic electrons and positrons passing through the thin and half-wave crystals, including mirroring; channeling radiation from electrons in a half-wave crystal; depth oscillations of electronuclear reactions caused by relativistic planar channeled electrons; optical radiation from channeled relativistic heavy ions in vicinity of the Cherenkov angle; angular distribution features of Channeling radiation in the optical range; PXRC (parametric X-Radiation at channeling) and its quantum features; radiation energy loss of channeled relativistic electrons in a crystal; positron source via electron-positron pair production by channeling radiation.

In the future we plan to make available the described packages for the channeling scientific community.

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