ELECTRON BEAM DYNAMICS AND CHANNELING RADIATION SIMULATION IN CRYSTAL

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2D code was designed for the simulation and simulation algorithms and methods are discussed in this report. The planar channeling is studying. Results of electron dynamics and radiation simulations are presented. The designed algorithm can be also used to separate channeled and dechanneled particles. The dependence of the oscillation period versus electron oscillation amplitudes is simulated. It allows defining of the radiation spectrum. The fundamental and high order harmonics radiation probability is discussed. The probability of radiation spectrums is presented.

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INTRODUCTION

The method of obtaining of the narrow-band X-rays lies in utilizing the principle of so called channeling radiation from crystals [1 - 3].

Channeling radiation is emitted by relativistic electrons passing through single crystals along a direction of high symmetry. The radiation is forward directed into a narrow cone with an angle of emission $\Theta \sim \gamma^{-1}$.

There are two different types of channeling dependent on the electron track – axial channeling and planar channeling [4]. In the first case electron captured in the channel is moving along the crystal axis and experience the influence of the axially-symmetrical averaged coulomb field of the crystal axis. In the planar channeling the particle is forced by the fields of the atoms situated on the crystalline plane.

The mechanism of channeling radiation can be described in two principal ways: classical physics model and quantum mechanics.

1. MAIN RELATIONS AND ANALYTICAL STUDY

Electrical field formed between the crystallographic planes forming the channel can be characterized with an averaged potential $U(x)$ where x is transversal offset from the channel central plane. As a rule $U(x)$ is smooth, even and periodical function with period of $2d$: $U(-x) = U(x)$, $U(x + 2dk) = U(x)$, where $2d$ is the channel width, k – integer number. Potential value on the border of the channel can be labeled as $U(|x| = d) = U_0$. Potential describing the electron channeling phenomenon is often called "reversed parabola" [3]. With fine accuracy it can be expressed as follows:

$$U(x) = U_0 \sum_{n=0}^{N} a_n \left(\frac{x}{d}\right)^n \quad |x| < d, \qquad (1)$$

where U_0 – potential of the field in crystal, $2d$ is the distance between the crystal planes.

The schematic view of such potential is shown in Fig. 1 for diamond crystal with U_0=23.6 V and d=0.67 Å.

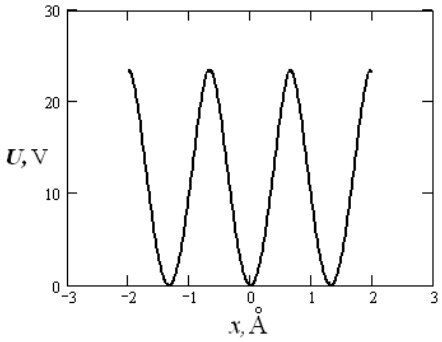

Fig. 1. Schematic view of crystal potential [4]

In this field the particle with charge e, energy ε and rest mass of m perform small transversal harmonic oscillations relative to channel central plane. If the magnitude of oscillations is much less then channel width ($x_m << d$) and the period of the oscillations can be expressed as:

$$\Omega_n = \sqrt{2\Omega_0}, \ \Omega_0 = \frac{c}{d}\sqrt{\frac{2eU_0}{\varepsilon}}, \qquad (2)$$

here $\gamma = \varepsilon / mc^2 = (1-\beta^2)^{-1/2}$ is reduced particle energy, $\beta = v/c$, v – particle velocity. It is obvious that the frequency of transversal oscillations is reduced with energy gain as $\sim \gamma^{-1/2}$ [4, 5].

Let us mention that the frequency of large transversal oscillations $x_m \sim d$ depends on their amplitude. Therewith in particle motion Fourier harmonic expansion appears higher harmonics of the fundamental frequency and the particles motion becomes anharmonic. This fact is significant for investigation of the radiation spectral characteristics

Radiation frequency of k-harmonic propagating with angle θ to the central plane of the channel in dipole approximation for ultra-relativistic motion ($\gamma >> 1$) can be written as:

$$\omega_k = \frac{2k\Omega\gamma^2}{1+\theta^2\gamma^2}, \quad (\theta << 1, \ \gamma >> 1). \qquad (3)$$

Radiation frequency achieves its maximum at the zero angle: $\omega_k = 2k\Omega\gamma^2$.

Based on mentioned equations maximum energy for 9 MeV electron channeling relative to (110) plane of the diamond crystal estimation value of the radiated X-ray

photons can be obtained. For this case maximum value appears to be ħω=5.90 keV that qualitatively matches with experimental results [3].

Power of radiation losses of electron due to channeling radiation is defined by the equation:

$$P = \frac{2e^4 < E^2 > \gamma^2}{3m^2 c}, \qquad (4)$$

here $< E^2 >$ is the mean square of electrical field along the particle trajectory.

In the general the spectral and angle distribution of the irradiated energy can be defined as the sum [5, 6]:

$$\frac{\mathrm{d}^2 \varepsilon}{\mathrm{d}\omega d\theta} = \frac{e^2}{\pi^2 c} \sum_{k=1}^{\infty} \frac{\left|\boldsymbol{a}_k(\omega,\theta,\varphi)\right|^2}{\Omega^2} \frac{\sin^2(\pi K \sigma_k)}{\sigma_k^2}. \qquad (5)$$

Here the vector $\boldsymbol{a}_k = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} \boldsymbol{a}(t) e^{ik\Omega t}\,\mathrm{d}t$,

$\boldsymbol{a}(t) = \left[\boldsymbol{n}\left[\boldsymbol{n} - \beta\right]\dot{\beta}\right](1 - \boldsymbol{n}\beta)^{-2} \exp\left[-\frac{i\omega}{c}\left(n_x x + n_y y + n_z \delta z\right)\right]$,

$\sigma_k(\omega,\theta) = \Omega^{-1}\left[\omega(1 - n_z\beta_z) - k\Omega\right]$, $n_x = \sin\theta\cos\varphi$, $n_y = \sin\theta\sin\varphi$, $n_x = \cos\theta$, θ is the angle of normal $\boldsymbol{n}$ and longitudinal axis z, φ is the angle of projection of $\boldsymbol{n}$ to (x, y) plane, vector $\boldsymbol{a}_k(\omega,\theta,\varphi)$ defines radiation characteristics versus electron oscillations form and amplitude.

In the dipole case for the ultra relativistic electron we can to simplify the equation for spectral and angle distribution and the irradiation spectrum can be defined from (5) as: $\boldsymbol{a}_k = \frac{\left[\boldsymbol{n}\left[\boldsymbol{n} - \beta\right]\dot{\beta}_k\right]}{(1 - \boldsymbol{n}\beta)^2}$, $\dot{\beta}_k = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} \dot{\beta} e^{ik\Omega t}\,\mathrm{d}t$, $\sigma_k = \Omega^{-1}\left[\omega' - k\Omega\right]$ and we can to write equation of the radiation energy spectrum

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}\xi} = \frac{8e^2\gamma^4}{c\Omega} \times \times \sum_{k=E(\xi+1)}^{\infty} \left|\dot{\beta}_k\right|^2 \frac{\sin^2(\pi K(u\xi - k))}{(u\xi - k)^2} \frac{1}{u^2}\left(1 - \frac{2}{u} + \frac{2}{u^2}\right)\mathrm{d}u, \qquad (6)$$

here $\xi = \omega / 2\Omega\gamma^2$.

For the very large number of structure periods as it is observed in crystal Eq. (6) can be rewritten as:

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}\xi} = \frac{8\pi^3 e^2 K \gamma^4}{c\Omega} \sum_{k=E(\xi+1)}^{\infty} \left|\dot{\beta}_k\right|^2 \frac{\xi}{k^2}\left(1 - \frac{2\xi}{k} + \frac{2\xi^2}{k^2}\right)\mathrm{d}u. \qquad (7)$$

The general view of electron phase trajectories in ideal crystal with a harmonic potential are shown in Fig. 2 [2].

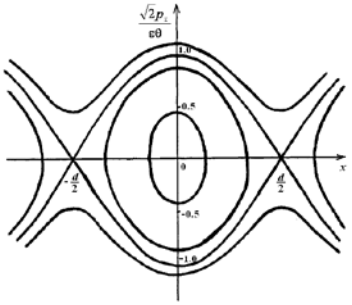

Fig. 2. Analytically predicted electron phase space trajectories in crystal with a harmonic potential [1]

2. CODE FOR NUMERICAL SIMULATION

The numerical simulation of electron oscillations in a crystal was performed for planar channeling. The equations of electron motion in a crystal in 2D Cauchy form are:

$$\begin{aligned} \frac{\mathrm{d}\gamma}{\mathrm{d}t} &= 0, \\ \frac{\mathrm{d}z}{\mathrm{d}t} &= v_z, \\ \frac{\mathrm{d}v_x}{\mathrm{d}t} &= -e\frac{\partial U(x)}{\partial x}, \\ \frac{\mathrm{d}x}{\mathrm{d}t} &= v_x. \end{aligned} \qquad (8)$$

Here $\gamma = W/W_0$ – Lorenz-factor. The crystal potential is presented in the generalized form Eq. 1, coefficients a_n define the form of the crystal potential and are known from numerous experimental data for a wide number of the most useful crystals. It is proposed in the model that the electron energy loss by radiation is much smaller than beam energy and may be neglected.

New code for electron motion simulation in a crystal was created using the BEAMDULAC code [7 - 9]. The BEAMDULAC beam dynamics simulation code includes a basic core and a number of modules. It was under development in DINUS research Laboratory at MEPhI for the many years. The code has the modular structure and numbers of routines to different task solve: initial particles distribution (uniformly, Gauss, waterbag), motion equation integration (4th order Runge-Kutta method), beam emittance calculation, post processing and etc. The code package has versions for own space charge effects treatment both Coulomb part and RF part (beam irradiation and beam loading).

The number of BEAMDULAC code modules (injection, integration, emittance calculation, post-processing) were used to solve the channeling of electrons in crystal problem.

Some modifications were made in the code to analyze results of the beam dynamics simulation of electrons in crystal. First we should define the oscillation period. It can be calculated as the distances between of two zeros of trajectories $\left|\tilde{x} - < x >\right|$. Second the phase trajectories ($\dot{\beta}_r$) of each particle were expanded to the Fourier series. The oscillations period of electron should be defined for it and Fast Fourier Transform (FFT) algorithm applying to define the oscillation harmonics. Following the averaged electron's energy loses to radiation are simulated as [5]:

$$< \delta W_{rad} > = \frac{r_0 l_{cr} \gamma^2}{3W_0} < E_{ch} >^2, \qquad (9)$$

where $< E_{ch} >$ is the averaged field acting to the electron, l_{cr} is the crystal length, $W_0 = mc^2$, $r_0 = e^2/4\pi\varepsilon_0 m^2 c^4 = 1.82 \cdot 10^{-15}$ m. The number of photons radiated by each electron can be calculated and the total number of generated photons can be defined to the each frequency.

3. EXAMPLES OF SIMULATION

The test simulation was made for diamond crystal having crystal potential U_0=23.6 V and coefficients a_1=4.0, a_3= -8.0, d=0.67 Å. The crystal length was chosen as 55 μm because of the multiple electrons scattering will influence sufficiently to results for thicker crystals.

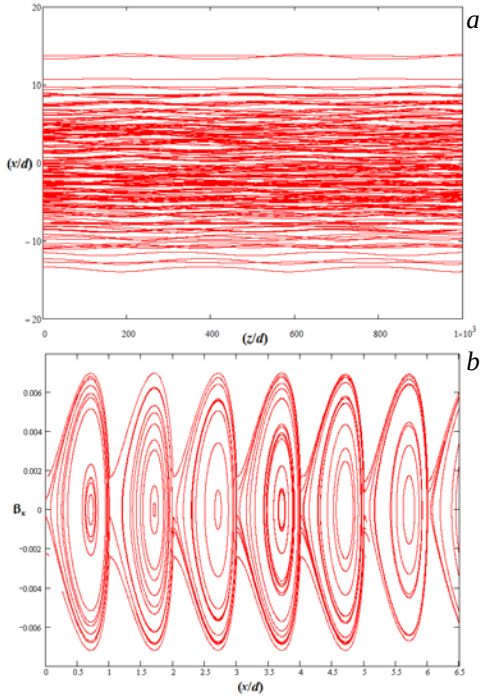

Fig. 3. Trajectories of channeled electrons in (z, x) plane (a) and phase trajectories in (β_r, r) phase plane (b) are shown

The results of simulation are presented in Fig. 3. The trajectories in (*z*, *r*) plane (a) and phase trajectories in (β_r, *r*) phase plane (b) are shown. The beam energy is 21 MeV, waterbag initial distribution was used for simulation. Trajectories in Fig. 3,a are detailed because of the number of oscillations is a thousands for 55 μm length crystal. The values of length and transverse coordinate are normalized: $\beta=v/c$, $\rho=x/d$. The phase motion stability region and the separatrix are clear seen. Note that the electrons phase trajectories in the crystal are similar to the analytically predicted (see Fig. 2 and [1]). Both the fundamental and the third spectrum harmonics can be seen from the figure.

The maximal angle of electron's trajectory and crystal plane θ_m can be easily defined with initial distribution conditions. An electron can be dechanneled in case when this angle will be bigger than critical angle θ_{cr}. As the first example the maximal injection angle is restricted by θ_m $2.5\cdot10^{-3}$ and the part of dechanneled electrons is about 7%.The dechanneling is more intensive in case when injection angle increased up to $7.5\cdot10^{-3}$. The part of dechanneled particles grows up to 30% this case (Fig. 4). Trajectories of unchanneled electrons can be easily seen in Fig. 4,a and they have the large angles with crystal planes and unstable phase trajectories in (β_r, *r*) phase plane are placed top and bottom of separatix. A dechanneled particle cross a number of channels. The oscillation period of such particles is much smaller than of channeled one. The multiple scattering of electrons moving in crystal close to the separatrix can brought to the particle dechanneling.

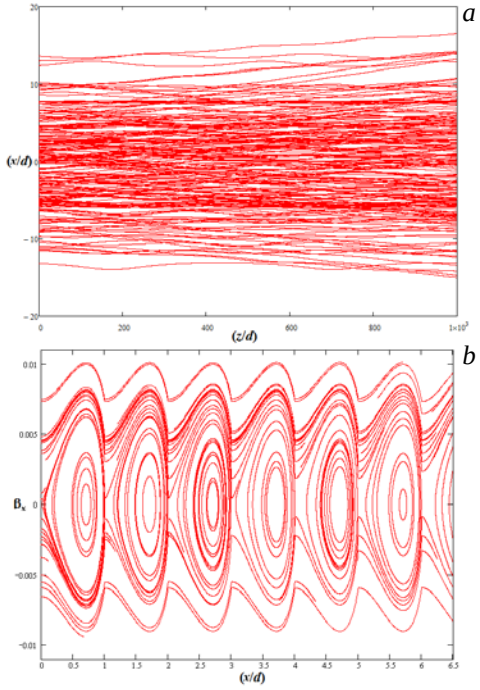

Fig. 4. Channeling of electrons in case of large value of injection angle θ, dechanneled particles can be seen

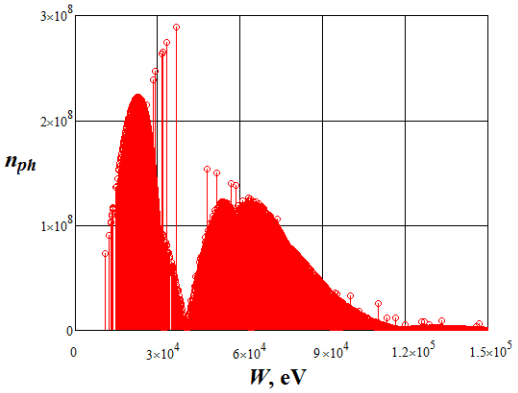

Fig. 5. Typical energy distribution of radiated photons

The total energy distribution of radiated photons n_{ph} is shown in Fig. 5. The distribution is calculated with W=21 MeV, injection angle is equal to $2.5\cdot10^{-3}$, number of electrons in the bunch is equal to $n_e=6\cdot10^{11}$ with corresponds to 1 mA of pulse beam current and 10 μs pulse length. Such bunch parameters are typical for electron linacs. The dechanneled particles are excludes from spectrum calculation after particles dynamics simulation by the simple algorithm. Following the probability of one electron radiation is calculating using known oscillation frequencies distribution and Eq. (4). At last the probability density distribution is multiplies on the particles number in the bunch.

The simulation shows that the frequency density distribution maximums are shifted right with electrons energy increase which corresponds to the theory.

If we can to define the phase trajectories of channeled electrons the period of oscillations can be calculated for all particles. The connection of electrons oscillation period T and amplitude x_{max} in crystal is shown in Fig. 6.

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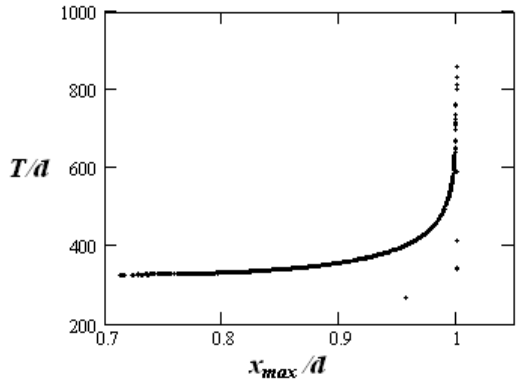

Fig. 6. Dependence of electrons oscillation period (T/d) of oscillation amplitude (x_{max}/d)

CONCLUSIONS

The oscillations of electrons in crystal are discussed in the effective potential approach. The general analytical description was presented and main predictions are made. Following the especially designed code to simulate electrons dynamics in crystal was discussed. Results of simulation are presented and they are very close to analytically proposed.

Let us discuss one possible channeling radiation application. Nowadays angiography has become one of the most commonly used medical procedures. However the X-ray tubes are mostly used in angiography imaging systems. The problem that encounters in using X-ray tubes is low monochromaticity due to bremsstrahlung while angiography imaging requires quasimonochromatic energy spectrum for better image quality and lower dose rate obtained by the patient. There are several methods of eliminating undesirable spectrum parts of the radiation: synchrotron or undulator radiation, Compton scattering, K-capture and radiations in aligned crystals (such as channeling radiation, coherent bremsstrahlung, parametric X-ray radiation, etc.).

The new angiography facility was proposed in [10]. The channeling radiation and polycapillary optics to prevent the irradiation of the patient by bremsstrahlung from crystal is proposed to utilize in such new facility.

REFERENCES

1. Yu.A. Bashmakov, E.G. Bessonov // *Rad. Eff.* 1982, v. 66, p. 85-94.
2. J. Freudenberger, H. Genz, L. Groening, et al. // *NIM B 119*. 1996, p. 123-130.
3. S.B. Dabagov, N.K. Zhevago // *Rivesta del nuovo cimento.* 2008, v. 31, № 9, p. 491-529.
4. J. Lindhard // *Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd.* 1965, v. 34, №14.
5. D.F. Alferov, Yu.A. Bashmakov, P.A. Cherenkov // *Sov. Phys. Usp.*. 1989, v. 32, p. 200; *Usp. Fiz. Nauk.* 1989, v. 157, p. 389 (in Russian).
6. D.F. Alferov, Yu.A. Bashmakov, E.G. Bessonov: Preprint LEBEDEV-72-23. 1972.
7. E.S. Masunov, S.M. Polozov // *NIM A.* 2006, v. 558, p. 184.
8. E.S. Masunov, S.M. Polozov // *Problems of Atomic Science and Technology. Series "Nuclear Physics Investigations"*. 2008, № 5, p. 136.
9. E.S. Masunov, S.M. Polozov // *Phys. Rev. ST AB.* 2008, v. 11, p. 074201.
10. Yu.A. Bashmakov, T.V. Bondarenko, S.M. Polozov, G.B. Sharkov // *Proc. of. RuPAC'2012*. 2012, p. 406.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ДИНАМИКИ И ИЗЛУЧЕНИЯ ЭЛЕКТРОННОГО ПУЧКА ПРИ КАНАЛИРОВАНИИ В КРИСТАЛЛЕ

Ю.А. Башмаков, С.М. Полозов

Описываются алгоритмы и численные методы, использованные при разработке программы для двумерного численного моделирования. Рассматривается случай плоскостного каналирования и приведены результаты моделирования динамики электронов в кристалле и сопровождающего излучения. Выделяются частицы, захваченные в канал, и частицы, совершающие надбарьерное движение. Определяется зависимость периода колебаний от начальных условий. Эта зависимость существенна для определения спектральных свойств излучения. Рассмотрена возможность генерации основной и высших гармоник излучения. Приводятся спектры вероятности излучения.

ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ ДИНАМІКИ І ВИПРОМІНЮВАННЯ ЕЛЕКТРОННОГО ПУЧКА ПРИ КАНАЛУВАННІ В КРИСТАЛІ

Ю.А. Башмаков, С.М. Полозов

Описуються алгоритми і чисельні методи, що були використані при розробці програми для двомірного моделювання. Розглядається випадок площинного каналування і наведені результати моделювання динаміки електронів у кристалі і супровідного випромінювання. Виділяються частинки, захоплені в канал, і частинки, що роблять надбар'єрний рух. Визначається залежність періоду коливань від початкових умов. Ця залежність істотна для визначення спектральних властивостей випромінювання. Розглянуто можливість генерації основної і вищих гармонік випромінювання. Приводяться спектри ймовірності випромінювання.