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SIMULATION OF THE RELATIVISTIC DYNAMICS OF CHARGED PARTICLES WITHIN THE ELECTROSTATIC PERIODIC FIELD OF PERFECT CRYSTALLINE UNDULATOR

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Abstract

The mathematical model of the passing of relativistic positrons within the interplanar space of positively charged crystalline structures composed of charged ellipsoids was received in this paper. The model includes the numerical-analytical models of both the electrostatic field potential of the structures and the electric intensity of the field as well as the numerical model of the relativistic positrons' dynamics in the field. The model of the field was received by the superposition principle. The case of the positrons passing through the long channel composed of charged ellipsoids, the centers of which are located in the nodal points of a three-dimensional lattice with a cubic unit cell, is considered. It was found the trajectories of positrons are close to sinusoidal on average for long intervals of time when the positrons move within the interplanar space of considered structures

Keywords

Channeling effect, electromagnetic radiation source, undulator, coherent radiation, electrostatic field, charged particles dynamics, mathematical simulation

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Introduction. X-ray and gamma-ray generators of coherent short-wave radiation (CSR) are of interest to a wide range of users. They should be useful and irreplaceable when studying the kinetics of chemical and biochemical reactions, the nature of viruses and bacteria, as well as progress in the limited possibilities of visual observation of process dynamics.

One of the possible ways of generating CSR, and currently the most successful one, is to use free-electron lasers (FEL). Such a laser is a device where two main elements are connected in series: 1) an accelerator of electrons (or positrons); 2) the so-called undulator — a long chain of sign-alternating magnetic or electric fields [1].

The accelerator generates a high-quality electron (or positron) beam, which, passing through the undulator along the "slalom" path, generates electromagnetic radiation. Because of relativistic effects, the radiation pattern is elongated in the direction of motion of the beam particles with an angular spread $\theta \sim 1/\gamma\sqrt{N_0}$, where γ is relativistic factor; N_0 is the number of undulator periods, and the longitudinal and transverse coherence $l_{||} \sim \lambda N_0$ and $l_{\perp} \sim \lambda/(2\pi)$ are respected.

The characteristics wavelength of the FEL accelerator is determined from the relation

$$\lambda = \frac{\lambda_0}{2\gamma a}\left(1 + \frac{\kappa^2}{2} + \gamma^2\theta^2\right) \approx \frac{\lambda_0}{2\gamma^2} \approx 0,13\frac{\lambda_0}{\varepsilon_e^2\left(\mathrm{MeV}\right)}, \tag{1}$$

where λ_0 is undulator period; $\kappa = \dfrac{eB\lambda_0}{2\pi m_e e} \cong 0,965B\lambda_0$ is undulatory coefficient; ε_e is the energy of the beam particles. If $\kappa \le 1$, for a sufficient length of the undulator, the radiation is coherent, its power due to the interaction of the beam particles with its electromagnetic field of radiation is proportional N_0^2, and the amplitude of the oscillations of the "slalom" movement is small. If $\kappa \ge 1$, the nature of the radiation changes: it will be incoherent, its power is proportional N_0, and the amplitude of the oscillations of the beam particles is large. Such a system of alternating fields by accepted terminology is called a wiggler.

The width of the spectral line in the undulator is estimated as $\Delta\lambda/\lambda \sim 1/2N_0$. Usually the number of periods of the undulator is large (hundreds and thousands), and the length of the undulator can exceed a hundred meters. If $N_0 \gg 1$, and a beam quality is sufficiently high $\Delta\varepsilon_e/\varepsilon_e \le 1/N_0$, then the beam particles are grouped into short bunches which oscillate as a whole in the field of their electromagnetic radiation, and the radiation itself becomes coherent.

To some extent, the classical collective vibrations of the bunch in the own field resemble the mechanism of the induced quantum-mechanical transition of the excited electrons of the atom to the ground state under the action of the intrinsic radiation of other atoms and, in fact, are its classic counterpart.

FEL gain factor

$$Gl = 7\cdot 10^{-4} I_e\left(a\right)\frac{N_0^2}{\gamma_e} \gg 1, \tag{2}$$

where $I_e(a)$ is beam current. Conditions (1) and (2) contradict each other. According to (1), to generate shorter wavelength radiation, it is necessary to increase the energy of the beam particles ($\gamma_e \gg 1$) and reduce the undulator period λ_0, and for larger values Gl, it is necessary to reduce the energy of the beam particles and increase the number of undulator periods.

Typical values of the wiggler period are several centimeters (≈ 3 cm), which determines the significant length of the undulator as a whole. For example, *The European X-Ray Free-Electron Laser* (*XFEL*) has a total length of about 3.4 km with one of three undulators approximately 210 m long. The *XFEL* X-ray wavelength is 0.05–4.70 nm, and the quantum energy of this radiation is 2.6–24.8 keV. The *XFEL* laser is capable of delivering up to 27.000 pulses per second with pulse duration of 30–100 fs. The accelerator gives electrons energy up to 17.5 GeV [2].

To advance even shorter waves, it is necessary either to increase the energy of the beam particles and the number of periods of the undulator, or to reduce the period λ_0. To reduce the period λ_0 over the past several decades, the idea of creating an effective crystalline undulator, the principle of which would be based on the channeling effect in crystals [3, 4].

The channeling effect consists in the fact that charged particles can penetrate into the crystal at substantially greater distances compared to the interatomic distance, moving in the interplanar space if, when a particle enters the crystal surface, the angle between the direction of motion of the particle and any direction (channel) along which there are no nodes of the crystal lattice in this crystal [5].

This effect is confirmed by many experimental and theoretical works. Classical channeling experiments include those in which any charged particles pass through the thin single crystal and fall on the detector [6], as well as experiments in which the path of particles (radioactive ions) is measured by sequentially removing thin layers of the crystal with measurement of the residual radioactivity. It is proved that in the general case the length of the penetration of particles into the crystal is greatly increased if the direction of particle incidence on the surface of the single crystal is close to the directions of open channels in the crystal [7].

The basic theoretical model of the effect is considered the Lindhardt model, which considers it as the result of irradiation of the crystal with fast particles at a small angle to crystallographic planes not exceeding the Lindhardt critical angle, which takes values of the order of micro rad for positively charged particles with an energy in the range of 100 GeV–1 TeV [8]. In this case, the effect can be considered in the framework of classical mechanics if we are talking about the movement of either relatively heavy particles (protons, ions) or relatively fast particles (relativistic and ultrarelativistic positrons and electrons), and the accuracy of this approximation increases with increasing energy of the particle [9].

The Lindhardt angular criterion [9] is introduced based on a model that considers the interaction of a channeled fast particle with atomic chains or atomic planes, since Coulomb collisions of a charged particle with atoms of the structure are correlated with each other. The motion of a particle *p*, with momentum velocity v and charge *Ze* at a small angle to the crystallographic planes is considered as motion in a transverse potential well with a depth U_0, formed by continuously averaged potentials of neighboring atomic planes [8–10]. Lindhardt's angular criterion is the limiting angle of the capture of an incident particle in a transverse potential well

$$\theta_L = \sqrt{\frac{2ZeU_0}{pv}}. \tag{3}$$

Thus, if the angle between the direction of motion of the particles of the beam and the direction of any open channel does not exceed the critical (3), then the beam of charged particles goes into channeling mode. Particles move in a quasi-electrostatic periodic field of positively charged ions of the crystal lattice in the most remote region of space. In this regard, channeled high-energy particles practically do not collide with the nuclei, passing at a distance of about half the interplanar distance from them, and for nuclear reactions, it is necessary to approach the particles at distances 4–5 orders of magnitude smaller than the considered interplanar length. This makes the loss of energy of the particle beam associated with nuclear transformations insignificant [5]. The channeled particles interact with the crystal lattice through elastic Coulomb collisions with ions of the structure, and their trajectories are close to "slalom" [5, 11]. This allows us to consider the crystal as an undulator, the period of which is only about 0.1 nm.

However, long-term studies have shown that the use of real single crystals as undulators is associated with many insurmountable obstacles. There are many factors due to which charged high-energy particles somehow get out of the channeling mode. The set of processes occurring in a real crystal, or leading to the exit of charged particles from the channeling mode, or significant energy loss of particles, is called the dechanneling process [12]. Including in an ideal single crystal, the main mechanism of energy loss of channeled particles is ionization loss due to its interaction with electrons. Passing through a crystal, a charged particle is elastically scattered by electrons, transferring a significant part of the energy to them, which is subsequently spent on the excitation and ionization of atoms [11].

To describe the process of dechanneling in an ideal single crystal, one can use the diffusion approximation [8, 12, 13], according to which, in the depth of the crystal, the fraction of channeled particles decreases exponentially with the length of the dechanneling along the channel length L_D. in the case of a direct single crystal for fast particles, $\gamma \gg 1$, can be expressed as

$$L_D = \frac{256 p v a_{TF} d}{9\pi^2 \left(\ln \frac{2m_e c^2 \gamma}{I} - 1 \right) z r_e m_e c^2}.$$

Here $a_{TF} \cong 0,8853 a_B Z^{-1/3}$ is Thomas — Fermi screening value, $a_B = \hbar^2 / \left(m_e e^2 \right)$ is Bohr radius; I is ionization voltage; $r_e = e^2 / \left(m_e c^2 \right)$ is classical electron radius. Since an exponential decrease in the fraction of channeled particles takes place only inside the crystal, a relaxation length of the order of $L_{rel} \cong 0,2 L_D$ [8, 14] and describing stable channeling near the crystal surface is introduced.

At present, the problem of dechanneling in the design of a crystalline undulator, as well as many others, does not allow us to consider it as an existing alternative to modern generators of short-wave radiation, and to switch to the generation of coherent radiation in the region of even shorter wavelengths.

A compromise between a conventional undulator and a crystal can be the use of undulator with a period of $0.03 \text{ m} \gg \lambda_0 \gg 0.1 \text{ nm}$. Thus, it is possible to use a system with a characteristic period of 0.1–0.2 cm through controlled periodic dipole fields. Such fields can be created using a system of ferroelectrics or ferromagnets if an ultrasonic wave is launched along the surface using an external generator. In this case, a periodic electric or magnetic field is formed above the surface of the ferroelectric or ferromagnet, acting on the electron (or positron) beam as a normal undulator, but with a period of only 0.1–0.2 cm [15]. Other design options for undulators with a short ($\lambda_0 \ll 3$ cm) period are possible.

In this work, the channeling effect, together with all its advantages, is considered as the basis for creating a system for converting the trajectories of charged high-energy particles to the “slalom” type. The ideal periodic structure, composed of any charged objects according to the principle of a crystal lattice, is considered as a source of a periodic electrostatic field, which underlies the principle of operation of the undulator. Thus, it is possible to avoid the problem of dechanneling in real crystals and take advantage of the channeling effect by working with structures with a characteristic period within $0.03 \text{ m} \gg \lambda_0 \gg 0.1 \text{ nm}$. The electrostatic field of the structure is interesting only in its interplanar space and the use of the approximation of the field of a single “ion”, taking into account its three linear sizes. Such an approximation will correspond to the fact that in the nodes of a three-dimensional grid, as “ions”, it is necessary to place resting and non-interacting positively charged ellipsoids having three linear parameters.

As a subject of study, we consider the electrostatic field inside an arbitrary periodic structure composed of charged ellipsoids, as well as the dynamics of relativistic charged particles in the field under study. *The purpose of this paper* is to build evidence that the trajectories of positively charged particles moving inside an arbitrary periodic structure composed of charged ellipsoids will be close to sinusoidal, as well as to obtain the form of the particle trajectories themselves and the characteristics of the electrostatic field. As a technique, we use the construction of a mathematical numerical model that includes the calculation of the characteristics of the electrostatic field inside the crystal and numerical simulation of the dynamics of relativistic charged particles in a given field.

Simulation of an electrostatic field. We will approximate the ion field by the field of a charged ellipsoid with three parameters a, b, c and a charge Q. We assume that the ellipsoids are oriented identically and are at rest, and the potential of the resulting field is calculated according to the superposition principle.

The calculation of the field potential of an ellipsoid is carried out using ellipsoidal coordinates. We associate with the center of the i-th ellipsoid, defined by the radius vector $\vec{\rho}_i$, a new Cartesian coordinate system. Let the observation point in the original Cartesian system be given by the radius vector $\vec{r}$, and in the system associated with the i-th ellipsoid be given by the radius vector $\vec{r}_i$.

Under the condition $a > b > c > 0$, the ellipsoidal coordinates are uniquely defined as the roots $u = \xi, \eta, \zeta$ of the cubic with respect to the u equation

$$\frac{x_i^2}{a^2+u} + \frac{y_i^2}{b^2+u} + \frac{z_i^2}{c^2+u} = 1. \tag{4}$$

Belonging to the interval $\xi \geq -c^2$, $-c^2 \geq \eta \geq -b^2$, $-b^2 \geq \zeta \geq -a^2$. Suppose that the condition $a > b > c > 0$ does not restrict generality since its fulfillment can be ensured by an additional transformation for the coordinate system $\vec{\rho}$.

The sought field potential has ellipsoidal symmetry, and when calculating it, only the root ξ, which is an analog of the radial coordinate in the ellipsoidal system, is of interest. We rewrite equation (4) as a polynomial

$$f(u) = u^3 + A_2u^2 + A_1u + A_0, \tag{5}$$

where

$$A_2 = a^2 + b^2 + c^2 - r_i^2;$$
$$A_1 = a^2b^2 + a^2c^2 + b^2c^2 - x_i^2\left(b^2 + c^2\right) - y_i^2\left(a^2 + c^2\right) - z_i^2\left(a^2 + b^2\right);$$
$$A_0 = a^2b^2c^2 - x_i^2b^2c^2 - y_i^2a^2c^2 - z_i^2a^2b^2.$$

We calculate the leading root $\xi \geq -c^2$ of equation (5) using the trigonometric Vieta formula for the cubic equation. The expression for this root will look like

$$\xi = -2\sqrt{S}\cos\left(\frac{1}{3}\left[\arccos\left(\frac{R}{\sqrt{S^3}}\right) + 2\pi\right]\right) - \frac{A_2}{3},$$
$$S = \frac{A_2^2 - 3A_1}{9},\quad R = \frac{2A_2^3 - 9A_2A_1 + 27A_0}{54}. \tag{6}$$

The potential of the i-th ellipsoid field is an elliptic integral of the first kind $\left[\xi_i, +\infty\right)$ within ξ or in the canonical form $\left[0, \psi_i\right]$, $\psi_i =$ $= \arcsin\sqrt{\left(a^2 - c^2\right)/\left(a^2 + \xi_i\right)}$ within ψ and being a solution of the Laplace equation in ellipsoidal coordinates:

$$\varphi_i = \frac{Q}{2}\int\limits_{\xi_i}^{+\infty}\frac{d\xi}{\sqrt{\left(\xi + a^2\right)\left(\xi + b^2\right)\left(\xi + c^2\right)}} = \frac{Q}{\sqrt{a^2 - c^2}}\int\limits_0^{\psi_i}\frac{d\psi}{\sqrt{1 - \dfrac{a^2 - b^2}{a^2 - c^2}\sin^2\psi}}. \tag{7}$$

The calculation of the integral (7), associated with the i-th ellipsoid for an arbitrary observation point $\vec{r}$ can be implemented numerically. Here we use the fourth-order parabola method with an error that decreases as $1/N_{\varphi_i}^4$, by nodal points $\psi_{im} = m\psi_i/N_{\varphi_i}$, $m = 1, \ldots, N_{\varphi_i} + 1$.

Simulation of the relativistic dynamics of channeled particles. It is necessary to construct a numerical solution to the Cauchy problem for given initial conditions $\vec{v}_0$ and $\vec{r}_0$ for the relativistic equation o dynamics with an electrostatic Coulomb force.

Taking into account the principle of superposition for field potentials of i-th ellipsoids and the integral expression (7), we can write the expression for the j-th component of the field gradient:

$$\frac{\partial\varphi}{\partial r_j} = -\frac{Q}{2}\sum_i\frac{\partial\xi_i/\partial r_j}{\sqrt{\left(\xi + a^2\right)\left(\xi + b^2\right)\left(\xi + c^2\right)}}. \tag{8}$$

Differentiating expression (6), we obtain expressions for the derivative $\partial\xi_i/\partial r_j$:

$$\frac{\partial\xi_i}{\partial r_j}=\sqrt{S}\left(2\sin\left[\varphi+\frac{2\pi}{3}\right]\frac{\partial\varphi}{\partial r_j}-\frac{1}{S}\cos\left[\varphi+\frac{2\pi}{3}\right]\frac{\partial S}{\partial r_j}\right)-\frac{1}{3}\frac{\partial A_2}{\partial r_j};$$

$$\varphi=\frac{1}{3}\arccos\left(\frac{R}{\sqrt{S^3}}\right),\quad \frac{\partial\varphi}{\partial r_j}=\frac{1}{\sqrt{S^3-R^2}}\left(\frac{R}{2S}\frac{\partial S}{\partial r_j}-\frac{1}{3}\frac{\partial R}{\partial r_j}\right);$$

$$\frac{\partial S}{\partial r_j}=\frac{2}{9}A_2\frac{\partial A_2}{\partial r_j}-\frac{1}{3}\frac{\partial A_1}{\partial r_j};\quad \frac{\partial R}{\partial r_j}=\left(\frac{1}{9}A_2^2-\frac{1}{6}A_1\right)\frac{\partial A_2}{\partial r_j}-\frac{1}{6}A_2\frac{\partial A_1}{\partial r_j}+\frac{1}{2}\frac{\partial A_0}{\partial r_j};$$

$$\frac{\partial A_k}{\partial r_j}=-2\begin{pmatrix} x-\rho_x & y-\rho_y & z-\rho_z \\ \left(b^2+c^2\right)\left(x-\rho_x\right) & \left(a^2+c^2\right)\left(y-\rho_y\right) & \left(a^2+b^2\right)\left(z-\rho_z\right) \\ b^2c^2\left(x-\rho_x\right) & a^2c^2\left(y-\rho_y\right) & a^2b^2\left(z-\rho_z\right)\end{pmatrix}_{kj}.$$

The relativistic equation of dynamics with an electrostatic Coulomb force is a system of three ordinary second-order nonlinear differential equations. The Cauchy problem for a system of equations solved with respect to the highest derivatives and rewritten as a system of six first-order equations has the form

$$\frac{d\vec{v}}{dt}=\vec{f}\left(\vec{r},\vec{v}\right),\quad \frac{d\vec{r}}{dt}=\vec{v},\quad \vec{v}\left(t_0\right)=\vec{v}_0,\quad \vec{r}\left(t_0\right)=\vec{r}_0;$$

$$f_x=-\frac{e}{m}\left(\frac{\partial\varphi}{\partial x}\left(1-\frac{v_x^2}{C^2}\right)-\frac{1}{C^2}\left(v_xv_y\frac{\partial\varphi}{\partial y}+v_xv_z\frac{\partial\varphi}{\partial z}\right)\right)\sqrt{1-\frac{v_x^2+v_y^2+v_z^2}{C^2}};$$

$$f_y=-\frac{e}{m}\left(\frac{\partial\varphi}{\partial y}\left(1-\frac{v_y^2}{C^2}\right)-\frac{1}{C^2}\left(v_yv_x\frac{\partial\varphi}{\partial x}+v_yv_z\frac{\partial\varphi}{\partial z}\right)\right)\sqrt{1-\frac{v_x^2+v_y^2+v_z^2}{C^2}};\qquad(9)$$

$$f_z=-\frac{e}{m}\left(\frac{\partial\varphi}{\partial z}\left(1-\frac{v_z^2}{C^2}\right)-\frac{1}{C^2}\left(v_zv_x\frac{\partial\varphi}{\partial x}+v_zv_y\frac{\partial\varphi}{\partial y}\right)\right)\sqrt{1-\frac{v_x^2+v_y^2+v_z^2}{C^2}}.$$

We solve the Cauchy problem (9) by the fourth-order Runge — Kutta method. We introduce a one-dimensional time grid with nodal points $t_n=n\tau$ and a time step $\tau=T/N_t$, T is where the final moment in time; N_t+1 is the number of nodal points. We distort the approximate values of the coordinate functions and velocities on the grid $v_i^n=v_i\left(t_n\right)$, $r_i^n=r_i\left(t_n\right)$, $i=x,\ y,\ z$, $n=0,\ldots,N_t$. The difference problem that approximates the solution of the Cauchy problem (9) on the constructed grid will have the following form (the expression $\left\{v_j^n+\tau k_{3,v_j}\right\}$ implies the set of arguments of the function numbered by the index $j=x,y,z$):

$$k_{1,v_i}=f_i\left(r_x^n,r_y^n,r_z^n,v_x^n,v_y^n,v_z^n,\right),\quad k_{1,r_i}=v_i^n;$$

$$k_{2,v_i}=f_i\left(\left\{r_j^n+\frac{\tau}{2}k_{1,r_j}\right\},\ \left\{v_j^n+\frac{\tau}{2}k_{1,v_j}\right\}\right),\quad k_{2,r_i}=v_i^n+\frac{\tau}{2}k_{1,v_i};$$

$$k_{3,v_i}=f_i\left(\left\{r_j^n+\frac{\tau}{2}k_{2,r_j}\right\},\ \left\{v_j^n+\frac{\tau}{2}k_{2,v_j}\right\}\right),\quad k_{3,r_i}=v_i^n+\frac{\tau}{2}k_{2,v_i};$$

$$k_{4,v_i}=f_i\left(\left\{r_j^n+\tau k_{3,r_j}\right\},\ \left\{v_j^n+\tau k_{3,v_j}\right\}\right),\quad k_{4,r_i}=v_i^n+\tau k_{3,v_i};$$

$$v_i^{n+1}=v_i^n+\frac{\tau}{6}\left(k_{1,v_i}+2k_{2,v_i}+2k_{3,v_i}+k_{4,v_i}\right);$$

$$r_i^{n+1}=r_i^n+\frac{\tau}{6}\left(k_{1,r_i}+2k_{2,r_i}+2k_{3,r_i}+k_{4,r_i}\right).$$

To control the convergence, we use the criterion of convergence in the norm calculated for the difference of the grid functions. We denote by $y^{2\tau}$ and y^{τ} the grid functions obtained at step 2τ and τ, where y means one or another grid function v_i or r_i. Let the trace of the exact solution of the differential problem on the grid 2τ is y^*, and the trace of the grid function y^{τ} on the same grid is $y^{(\tau)}$. Now introducing one of the possible norms for the rid functions $y^{2\tau}$ and y^{τ} we have the convergence estimate

$$\left\|y^{(\tau)}-y^*\right\|\approx\frac{\left\|y^{2\tau}-y^{\tau}\right\|}{15}\le\varepsilon, \tag{10}$$

where ε is desired precision.

Simulation. Let $n=\left\{n_x,n_y,n_z\right\}$ determine the number of nodal planes of a three-dimensional grid along the corresponding axis of the Cartesian system, $T=\left\{T_x,T_y,T_z\right\}$ are three linear periods of a three-dimensional lattice. We place the center of symmetry of the periodic structure at the beginning of the Cartesian coordinate system and calculate the characteristics of the electrostatic field of the elementary channel $n=\left\{2,200,2\right\}$, $T=\left\{1\ \text{nm},\ 1\ \text{nm},\ 1\ \text{nm}\right\}$ in the region $x\in\left\{-1\ \text{nm},\ 1\ \text{nm}\right\}$, $y\in\left\{-1.5\ \text{nm},\ 1.5\ \text{nm}\right\}$, $z=0$ on a grid with step characteristics $h_x=h_y=0.02$ nm and at $N_{\varphi_i}=50$. Further, the characteristics of ellipsoids their charges are everywhere taken equal to $a=0.3$ nm, $b=0.25$ nm, $c=0.2$ nm, $Q=40e$. The results of calculating the level lines for scalar potential fields and two components of the strength E_x and E_y of the electrostatic field are shown in Fig. 1.

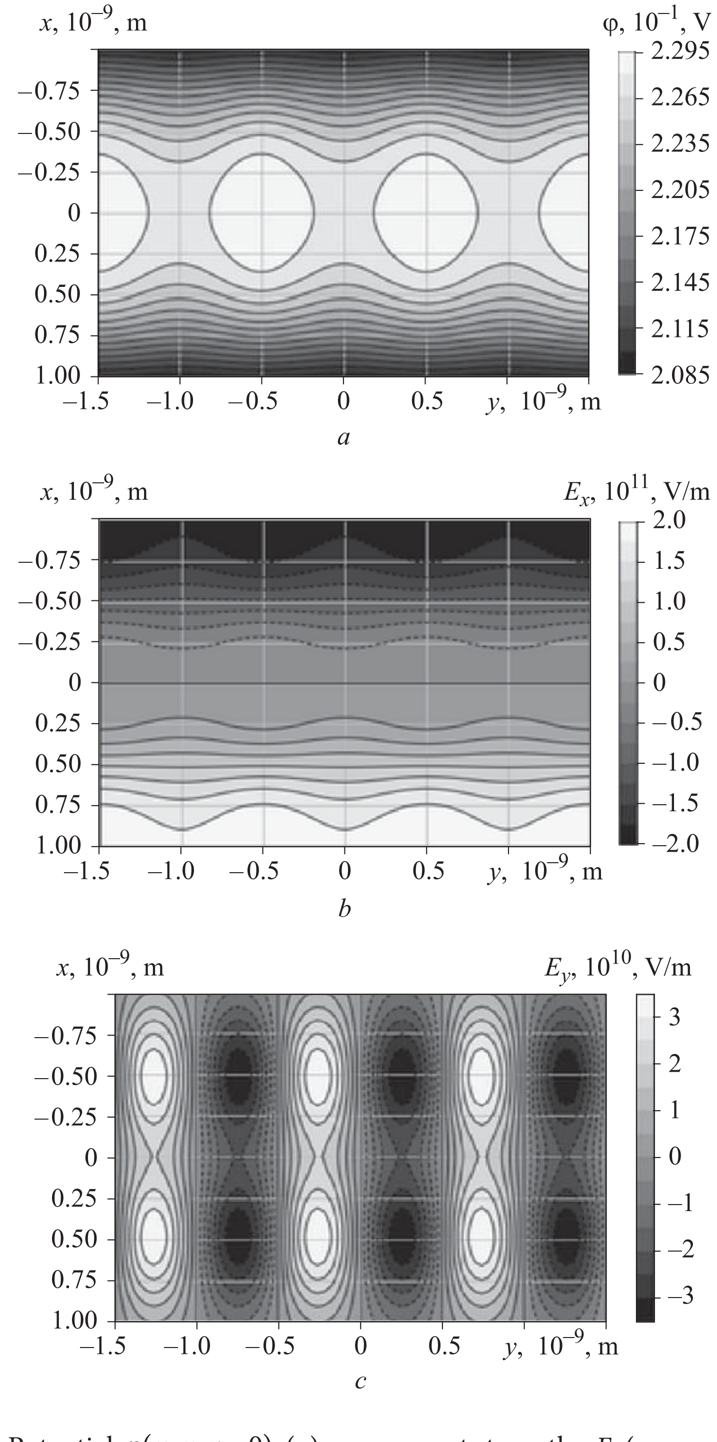

Fig. 1. Potential $\varphi(x, y, z=0)$ (a), component strengths $E_x(x, y, z=0)$ (b) and $E_y(x, y, z=0)$ (c) electrostatic field of the elementary channel

We turn to simulate the dynamics of the positron. Further, 1 nm is universally accepted as a unit of length, and 1 fs per unit of time. Thus, for the speed of light, we take the value 299.8 nm/fs. Set the initial coordinates and velocities for the positron as $\vec{r}_0 = \{0, -10, 0.1\}$, $\vec{v}_0 = \{0, 290, 0\}$ consider an elementary channel whose characteristics are set equal to $n = \{2, 1500, 2\}$, $T_x = T_y = T_z = 1$, whose nodal points are located symmetrically with respects to the Oz and Ox, its origin has a coordinate $y = 0$. The function graphs $y(t)$, $z(t)$, $v_y(t)$, $v_z(t)$, obtained as a numerical solution of the Cauchy problem (9) in the time interval 0–5.2 with accuracy (10) $\varepsilon = 0.05$ are shown in Fig. 2.

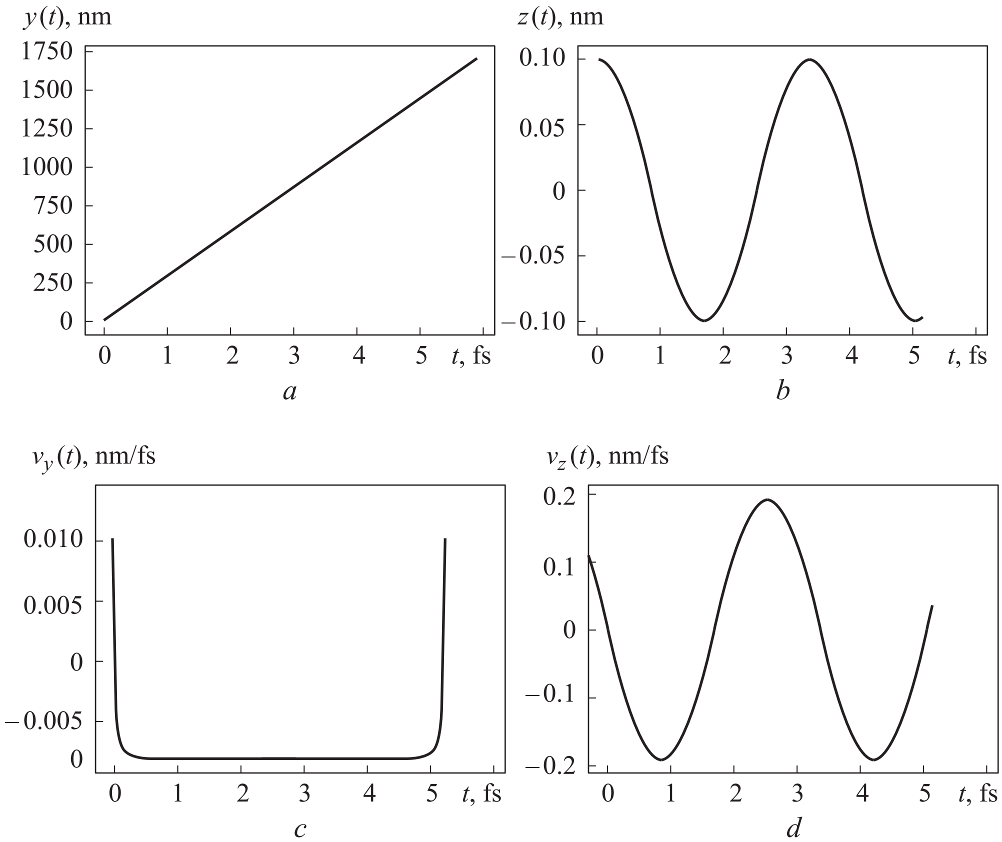

Fig. 2. The function graphs $y(t)$ (a), $z(t)$ (b), $v_y(t)$ (c) and $v_z(t)$ (d)

Due to a large number of oscillations, only the envelopes of the corresponding functions can be observed in the constructed graphs. In this case, the total radiation energy in the relativistic interpretation is composed, first of all, of the contributions corresponding to the regions with the smallest instantaneous radius of curvature of the trajectory. This follows from a comparison of the total radiation power for the case of rectilinear motion of a charge and instantaneous movement of a charge around a circle:

$$P_r\left(t'\right)=\frac{2e^2}{3m^2c^3}\left(\frac{dp}{dt}\right)^2, \quad P_{in}\left(t'\right)=\frac{2e^2}{3m^2c^3}\gamma^2\left(\frac{d\vec{p}}{dt}\right)^2.$$

For the v_y, v_z velocity components and y and z coordinate functions, the amplitude of the oscillations is small compared with the change in these values during the observation time, which allows one to see the form of the averaged functions $\langle v_y(t)\rangle$, $\langle v_z(t)\rangle$, $\langle y(t)\rangle$, $\langle z(t)\rangle$. We can conclude that these functions are approximately

$$\langle v_y(t)\rangle \approx \frac{B_1}{\left(B_2-\left(t-\tau\right)^{2s}\right)^b}; \quad \langle v_z(t)\rangle \approx B_{v_z}\sin\omega t;$$

$$\langle y(t)\rangle \approx \tilde{v}_y t; \qquad \langle z(t)\rangle \approx B_z\cos\omega t,$$

where values B_1, B_2, $m\in\mathbb{Z}^+$, $b>0$, $\tau>0$ are to be determined, and the rest take the values $B_{v_z}\approx 0.19$ nm/fs, $B_z = r_{0,z}=0.1$ nm, $\tilde{v}_y\approx 290$ nm/fs, $\omega = 2\pi/T$, $T\approx 4.25$ fs. The period of macroscopic oscillations of $T\approx 4.25$ fs corresponds to the passage of a positron through a layer of approximately 1226 elementary transverse panes of the channel, each of which contains four ellipsoids, i.e., the positron performs one complete macroscopic oscillation along the length $\lambda\approx 1226$ nm.

Conclusion. A mathematical model is constructed that allows modeling the electrostatic field of an arbitrary three-dimensional periodic structure composed of charged ellipsoids, as well as numerically calculating the relativistic dynamics of charged particles in a given field.

The constructed model was used as a tool in simulation the periodic electrostatic field of an undulator with a characteristic period $\lambda_0 \ll 3$ cm, as well as in simulation the dynamics of a relativistic positron in the field of such an undulator. It has been established that the trajectories of relativistic positrons moving in the interplanar space in the electrostatic field of an elementary channel composed of charged ellipsoids according to the periodic law on average over large periods are close to sinusoidal.

Translated by K. Zykova

REFERENCES

[1] Marshall T.C. Free-electron lasers. Macmillan, 1985.

[2] Branlard J., Ayvazyan G., Ayvazyan V., et al. The European XFEL LLRF system. *Proc. IPAC 2012*, 2012, MOOAC01, pp. 55–57.

[3] Korol A.V., Solov'yov A.V., Greiner W. Channeling of positrons through periodically bent crystals: on feasibility of crystalline undulator and gamma-laser. *Int. J. Mod. Phys. E*, 2004, vol. 13, no. 5, pp. 867–916. DOI: https://doi.org/10.1142/S0218301304002557

[4] Korol A.V., Solov'yov A.V., Greiner W. Photon emission by an ultra-relativistic particle channeling in a periodically bent crystal. *Int. J. Mod. Phys. E*, 1999, vol. 8, no. 1, pp. 49–100. DOI: https://doi.org/10.1142/S0218301399000069

[5] Tompson M. The channeling of particles in crystals. *UFN*, 1969, vol. 99, no. 2, pp. 297–317 (in Russ.). DOI: https://doi.org/10.3367/UFNr.0099.196910d.0297

[6] Nelson R.S., Thompson M.W. The penetration of energetic ions through the open channels in a crystal lattice. *Phil. Mag.*, 1963, vol. 8, no. 94, pp. 1677–1690.
DOI: https://doi.org/10.1080/14786436308207330

[7] Kumakhov M.A. Spatial redistribution of a flux of charged particles in a crystal lattice. *Sov. Phys. Usp.*, 1975, vol. 18, no. 3, pp. 203–221.
DOI: https://doi.org/10.1070/PU1975v018n03ABEH001954

[8] Biryukov V.M., Kotov V.I., Chesnokov Yu.A. Steering of high-energy charged-particle beams by bent single crystals. *Phys.-Usp.*, 1994, vol. 37, no. 10, pp. 937–960.
DOI: https://doi.org/10.1070/PU1994v037n10ABEH000048

[9] Lindhard J. Influence of crystal lattice on motion of energetic charged particles. *Mat.-Fys. Medd. Dan. Vid. Selsk.*, 1965, vol. 34, no. 1, p. 64.

[10] Matyukhin S.I. Critical parameters of channeling. *Tech. Phys.*, 2008, vol. 53, iss. 12, pp. 1578–1585. DOI: https://doi.org/10.1134/S1063784208120074

[11] Denisov S.P. Ionization energy loss of charged particles. *SOZh*, 1999, vol. 5, no. 11, pp. 90–96 (in Russ.).

[12] Kadmenskiy A.G., Samarin V.V., Tulinov A.F. Regular and statistical motion in a crystal at channeling. Evolution of the particle flux in a thick crystal. *EChAYa* [Physics of Elementary Particles and Atomic Nuclei], 2003, vol. 34, no. 4, pp. 822–868 (in Russ.).

[13] Zhevago N.K., Glebov V.I. Channeling and electromagnetic radiation of relativistic charged particles in metal-organic frameworks. *J. Exp. Theor. Phys.*, 2017, vol. 124, iss. 6, pp. 845–853. DOI: https://doi.org/10.1134/S1063776117060176

[14] Gemmell D.S. Channeling and related effects in the motion of charged particles through crystals. *Rev. Mod. Phys.*, 1974, vol. 46, iss. 1, pp. 129–235.
DOI: https://doi.org/10.1103/RevModPhys.46.129

[15] Vysotskiy V.I., Kuzmin R.N. Gamma-lazery [Gamma-lasers]. Moscow, MSU Publ., 1989.

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