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Stable propagation of a modulated positron beam in a bent crystal channel

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Abstract
The propagation of a modulated positron beam in a planar crystal channel is investigated. It is demonstrated that the beam preserves its modulation at sufficiently large penetration depths, which opens the prospect of using a crystalline undulator as a coherent source of hard x-rays. This finding is a crucial milestone in developing a new type of laser radiating in the hard x-ray and gamma-ray range.

(Some figures in this article are in colour only in the electronic version)

In this communication we study for the first time the evolution of a modulated particle beam in a bent planar crystal channel and demonstrate that a positron beam preserves its modulation at sufficiently large penetration depths, which opens the prospect of using a crystalline undulator as a coherent source of hard x-rays. Solving this problem is of crucial importance in the theory of the crystal undulator-based laser (CUL) [1–3]—a new electromagnetic radiation source in hard x- and gamma-ray range.

Channelling takes place if charged particles enter a single crystal at small angle with respect to crystallographic planes or axes [4]. The particles get confined by the interplanar or axial potential and follow the shape of the corresponding planes and axes. This suggested the idea [5] of using bent crystals to steer the particle beams. Since its first experimental verification [6] the idea to deflect or extract high-energy charged particle beams by means of tiny bent crystals replacing huge dipole magnets has been attracting a lot of interest worldwide. Bent crystals have been routinely used for beam extraction in the Institute for High Energy Physics, Russia [7]. A series of experiments on the bent crystal deflection of proton and heavy ion beams was performed at different accelerators [8–12] throughout the world. The bent crystal method has been proposed to extract particles from the beam halo at CERN’s Large Hadron Collider [13]. The possibility of deflecting positron [14] and electron [12, 15] beams has been studied as well.

A single crystal with periodically bent crystallographic planes can force channelling particles to move along nearly sinusoidal trajectories and radiate in the hard x- and gamma-ray frequency range (see figure 1). The feasibility of such a device, known as the ‘crystalline undulator’, was demonstrated theoretically a decade ago [1] (further developments as well as historical references are reviewed in [16]). More recently, an electron-based crystalline undulator has been proposed [17].

It was initially proposed to obtain sinusoidal bending by the propagation of an acoustic wave along the crystal [1, 2]. The advantage of this approach is its flexibility: the period of deformation can be chosen by tuning the frequency of the ultrasound. However, this approach is rather challenging technologically and yet to be tested experimentally. Several other technologies for the manufacturing of periodically bent crystals have been developed and tested. These include making regularly spaced grooves on the crystal surface either by a diamond blade [18, 19] or by means of laser-ablation [20], deposition of periodic Si\(_3\)N\(_4\) layers onto the surface of Si crystal [19], growing of Si\(_{1-x}\)Ge\(_x\) crystals [21] with a periodically varying Ge content [22, 23].

Experimental studies of the crystalline undulator are currently in progress. The first results are reported in [24] and [25].
lasing regime of the crystalline place in a crystalline undulator, it can be referred to as the
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the wavelength of the produced radiation
magnitude smaller than that of a conventional undulator. Therefore
hundreds or tens of micron which is two to three orders of mag-
reaches the (sub)picometre range, where conventional sources with comparable intensity are unavailable [26].

Even more powerful and coherent radiation will be emitted if the probability density of the particles in the beam is modulated in the longitudinal direction with the period
, equal to the wavelength of the emitted radiation. In
this case, the electromagnetic waves emitted in the forward
direction by different particles have approximately the same
phase [27]. Therefore, the intensity of the radiation becomes
proportional to the beam density squared (in contrast to
the linear proportionality for an unmodulated beam). This
increases the photon flux by orders of magnitude relative to
the radiation of unmodulated beam of the same density. The
radiation of a modulated beam in an undulator is a keystone
of the physics of free-electron lasers (FEL) [28, 29]. It can be
considered as the classical counterpart of stimulated emission
in quantum physics. Therefore, if a similar phenomenon takes
place in a crystalline undulator, it can be referred to as the
lasing regime of the crystalline undulator.

The feasibility of CUL radiating in hard x-ray and gamma-ray range was considered for the first time in [1, 2]. Recently,
a two-crystal scheme, the gamma klystron, has been proposed [3].

A simplified model used in the cited papers assumed
that all particle trajectories follow exactly the shape of the
bent channel. In reality, however, the particle moving along
the channel also oscillates in the transverse direction with
respect to the channel axis (see the shape of the trajectory
in figure 1). Different particles have different amplitudes of
the oscillations inside the channel (figure 2, upper panel).
Similarly, the directions of particle momenta in the (xz)
plane are slightly different (figure 2, lower panel). Even
if the speed of the particles along their trajectories is the
same, the particles oscillating with different amplitudes or
the particles with different trajectory slopes with respect to the
z axis have slightly different components of their velocities
along the channel. As a result, the beam gets demodulated.

An additional contribution to the beam demodulation comes
from incoherent collisions of the channelling particles with the
crystal constituents.

In the case of an unmodulated beam, the length of the
crystalline undulator and, consequently, the maximum
accessible intensity of the radiation are limited by the
dechannelling process. The channelling particle gradually
attains the energy of transverse oscillation due to collisions
with crystal constituents. At some point this energy exceeds
the maximum value of the interplanar potential and the particle
leaves the channel. The average penetration length at which
this happens is known as the dechannelling length. The
dechannelled particle no longer follows the sinusoidal shape
of the channel and, therefore, does not contribute to the undulator
radiation. Hence, the reasonable length of the crystalline
undulator is limited to a few dechannelling lengths. A longer
crystal would attenuate rather than produce the radiation.

Since the density of the undulator radiation is proportional to
the undulator length squared, the dechannelling length and the
attenuation length are the main restricting factors that have to
be taken into account when the radiation output is calculated.

In contrast, not only the shape of the trajectory but
also the particle positions with respect to each other along
the z axis are important for the lasing regime. If these
positions become random because of the beam demodulation,
the intensity of the radiation drops even if the particles are still
in the channelling mode. Hence, it is the beam demodulation
rather than dechannelling that restricts the intensity of the
radiation of CUL. Understanding this process and estimating
the characteristic length at which this phenomenon takes place
is, therefore, a cornerstone of the theory of this new radiation
source.

Let us consider the distribution 
 of the
beam particles with respect to the angle between the particle
trajectory and the $z$ axis in the $(x, z)$ plane $\xi = \arcsin p_x/p \approx p_x/p$ and the energy of the channelling oscillation $E_y = p_y^2/(2E) + U(y)^3$. Here $p_x$, $p_y$, and $p_z$ are, respectively, the particle momentum and its $x$ and $y$ components, $U(y)$ is the interplanar potential which in the case of positive particles, which channel between the crystallographic planes, can be approximated by a parabola $U(y) = \max(y/\max)^2$ and $E$ is the particle energy (we will consider only ultrarelativistic particles, therefore $E \approx p$). It can be shown that the evolution of this distribution in the crystal channel with the time $t$ and the longitudinal coordinate (penetration depth into the crystal along the curved channel) $s$ can be described by the following differential equation of Fokker–Planck type:

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial s} v_s = D_0 \left[ \frac{\partial}{\partial E_y} \left( E_y \frac{\partial f}{\partial E_y} \right) + \frac{1}{E} \frac{\partial^2 f}{\partial E^2} \right]. \quad (1)$$

Here $D_0$ is the diffusion coefficient that is dominated by the scattering of the beam particles by lattice electrons. The particle longitudinal velocity averaged over the undulator period, $v_s$, is given by

$$v_s = \left( 1 - \frac{1}{2\gamma^2} \frac{\xi^2}{2} \frac{E}{E^2} \right). \quad (2)$$

Equation (1) is akin to the equation describing dechannelling distribution can be represented as a Fourier series:

$$f(t, s, \xi, E_y) = \sum_{j=-\infty}^{\infty} g_j(s; \xi, E_y) \exp(i\omega t). \quad (3)$$

with $g_j(s; \xi, E_y)$ to ensure the real value of the particle distribution. Since equation (1) is linear, it is sufficient to consider only one harmonic. Substituting $f(t, s, \xi, E_y) = g(s; \xi, E_y) \exp(\omega t)$ one obtains

$$i\omega g(s; \xi, E_y) + \frac{\partial g}{\partial s} v_s = D_0 \left[ \frac{\partial}{\partial E_y} \left( E_y \frac{\partial g}{\partial E_y} \right) + \frac{1}{E} \frac{\partial^2 g}{\partial E^2} \right]. \quad (4)$$

To simplify this equation, we make the substitution $g(s; \xi, E_y) = \exp(-i\omega t) \hat{g}(s; \xi, E_y)$ and assume that the variation of $\hat{g}(s; \xi, E_y)$ within the modulation period is small: $\partial \hat{g}/\partial s \ll \omega \hat{g}(s; \xi, E_y)$. This allows us to neglect the terms $(1 - v_s)\partial \hat{g}/\partial s$ while keeping the terms $(1 - v_s)\omega \hat{g}(s; \xi, E_y)$. The resultant partial differential equation for $\hat{g}(s; \xi, E_y)$ can be solved by the method of separation of variables. Putting $\hat{g}(s; \xi, E_y) = S(s) \Xi(\xi) \hat{E}(E_y)$, we obtain a set of ordinary differential equations:

$$\frac{D_0}{\Xi(\xi)} \frac{d^2 \Xi(\xi)}{d\xi^2} - \frac{\xi^2}{2} = C_\xi, \quad (5)$$

We chose the system of units in such a way that the speed of light is equal to unity. Therefore, mass, energy and momentum have the same dimensionality. This is also true for length and time.

$$\frac{D_0}{\Xi(\xi)} \frac{d^2 \Xi(\xi)}{d\xi^2} = \frac{\xi^2}{2} = C_\xi, \quad (6)$$

$$\frac{1}{S(s)} \frac{dS(s)}{ds} + \frac{i\omega}{2\gamma^2} = C_s, \quad (7)$$

where $C_s$, $C_\xi$ and $C_\xi$ do not depend on any of the variables $s$, $\xi$ and $E_y$ and satisfy the condition

$$C_s = C_\xi + C_\xi. \quad (8)$$

Equation (5) has the form of the Schrödinger equation for the harmonic oscillator. Its eigenvalues and eigenfunctions are, respectively,

$$C_{\xi,n} = -(1 + i) \sqrt{\frac{\omega D_0}{E}} \left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots \quad (9)$$

and

$$\Xi_n(\xi) = H_n \left( \frac{\sqrt{\omega E}}{\sqrt{2D_0}} \xi \right) \exp \left( \frac{1 + i}{4} \sqrt{\frac{\omega E}{D_0}} \xi^2 \right). \quad (10)$$

Here $H_n(\cdots)$ are the Hermite polynomials.

Equation (6) can be reduced to the Laguerre differential equation, so that its solution can be represented as

$$L_k(\xi, E_y) = \exp \left( -\frac{1 + i}{2} \sqrt{\frac{\omega}{D_0 E}} \xi \right) L_{\nu_0} \left( 1 + i \sqrt{\frac{\omega}{D_0 E}} \xi \right) \quad (11)$$

where $L_\nu(\cdots)$ is the Laguerre function and $\nu_k$ is related to the eigenvalue $C_{\gamma, k}$ via

$$C_{\gamma, k} = -(1 + i) \sqrt{\frac{D_0 \omega}{E}} (2\nu_k + 1), \quad k = 1, 2, 3, \ldots. \quad (12)$$

The eigenvalues can be found by imposing the boundary conditions. The maximum energy of channelling oscillations in a bent channel with parabolic potential is given by $E_y = \max(1 - C)^2$, where $C = F_c/F_{\max}$ is defined as a ratio of the centrifugal force $F_c$ to the maximum value of the interplanar force $F_{\max}[16]$. Therefore, the density boundary condition has the form

$$L_{\nu_k} \left( 1 + i \sqrt{\frac{\omega}{D_0 E}} \max(1 - C)^2 \right) = 0. \quad (13)$$

Equation (13) has to be solved for $\nu_k$ (the subscript $k$ enumerates different roots of the equation) and the result has to be substituted into (12).

It is convenient to represent the eigenvalues in the form

$$C_{\gamma, k} = \frac{\alpha_k(\kappa, C)}{L_d} - i\omega \theta_k^2 \beta_k(\kappa, C). \quad (14)$$

Here $L_d = 4U_{\max}/(\beta_0 D_0)$ is the dechannelling length in a straight channel [30] ($\beta_0$ is 4th zero of the Bessel function $J_0(\epsilon)$ and $\theta_k = \sqrt{2U_{\max}/E}$ is the corresponding Lindhard’s angle. We introduce the parameter

$$\kappa = \frac{L_d \theta_k^2}{\lambda L}. \quad (15)$$

$^3$ At nonnegative integer values of $n$, the Laguerre function is reduced to the well-known Laguerre polynomials. In the general case that is relevant to our consideration, it can be represented by an infinite series: $L_\nu(\epsilon) = \sum_{n=0}^{\infty} \frac{(m - \nu)!}{m!} \epsilon^m / (m!)^2$. 

$^4$ The eigenfunctions of the harmonic oscillator are the Hermite polynomials $H_n$. They are orthogonal and eigenfunctions of the operator $\partial^2/\partial \xi^2 - \xi^2/2$.
where $\lambda = 2\pi/\omega$ is the spatial period of the modulation. The functions $\alpha_k(\kappa, C)$ and $\beta_k(\kappa, C)$ can be represented as

$$\alpha_k(\kappa, C) = \frac{\alpha_k(1 - C)^2}{(1 - C)^2}$$

$$\beta_k(\kappa, C) = (1 - C)^2 \beta_k(1 - C)^2.$$  

Here $\alpha_k(\kappa) \equiv \alpha_k(\kappa, C = 0)$ and $\beta_k(\kappa) \equiv \beta_k(\kappa, C = 0)$ are the corresponding functions for the straight channel which are found by solving numerically equation (13) combined with (12).

Using (8), one finds the solution of equation (7):

$$S_{n,k}(s) = \exp \left\{ -\frac{s}{L_d} \left[ \alpha_k(\kappa, C) + (2n + 1)\sqrt{\frac{\kappa}{j_{01}}} \right] \right\}$$

$$- i\omega s \left[ \frac{1}{2}\sqrt{\gamma} + \beta_k^2(\kappa, C) + \frac{1}{2}\sqrt{\gamma} \right]$$

Hence, the solution of equation (4) is represented as

$$g(s; \xi, E_y) = \exp(-i\omega s) \sum_{n=0}^{\infty} \sum_{k=1}^{\infty} c_{n,k} Z_n(\xi) E_y(s) S_{n,k}(s),$$

where the coefficients $c_{n,k}$ are found from the particle distribution at the entrance of the crystal channel. Due to the exponential decrease of $S_{n,k}(s)$ with $s$ (see (18)), the asymptotic behaviour of $g(s; \xi, E_y)$ at large $s$ is dominated by the term with $n = 0$ and $k = 1$ having the smallest value of the factor $[\alpha(\kappa, C) + (2n + 1)/j_{01}]$ in the exponential. Therefore, at sufficiently large penetration depths, the particle distribution depends on $s$ as $g(s; \xi, E_y) \propto \exp(-s/L_{dm} - i\omega/\upsilon_s s)$ where $L_{dm}$ is the newly introduced parameter—the demodulation length:

$$L_{dm} = \frac{L_d}{\alpha_1(\kappa, C) + \sqrt{\gamma}/j_{01}}$$

and $\upsilon_s$ is the phase velocity of the modulated beam along the crystal channel

$$\upsilon_s = \left[ 1 + \frac{1}{2}\gamma + \beta_k^2 \left( \frac{\beta_k(\kappa, C) + 1}{2j_{01}\sqrt{\gamma}} \right) \right]^{-1}.$$

This parameter is important for establishing the resonance conditions between the undulator parameters and the radiation wavelength. It will be analysed elsewhere.

In this communication we concentrate our attention on the demodulation length. It represents the characteristic scale of the penetration depth at which an initially modulated beam of channelling particles becomes demodulated.

Figure 3 presents the dependence of the ratio $L_{dm}/L_d$ on the parameter $\kappa$. At $\kappa \to 0$, the demodulation length approaches $(1 - C)^2 L_d$ which is the dechannelling length in the bent crystal. It was proven for a number crystal channels [16] that the dechannelling length of positrons is sufficiently large to make the crystalline undulator feasible. Such a crystalline undulator becomes a CUL, i.e. it generates coherent radiation, provided that it is fed by a modulated positron beam and the beam preserves its modulation over the length of the crystal. This takes place if the demodulation length in the crystalline undulator is not much smaller than the dechannelling length. As is seen from the figure, the demodulation length is smaller than the dechannelling length by only 20–30% at $\kappa \lesssim 1$ for $C$ varying between 0 and 0.3. It noticeably drops, however, at $\kappa \gtrsim 10$. Hence, CUL is feasible if there exist crystal channels ensuring $\kappa \lesssim 1$ in the range of the photon energies above ~100 keV.

Indeed, such crystal channels do exist. Figure 4 shows the dependence of the parameter $\kappa$ on the energy of the emitted photons $h\omega = 2\pi h/\lambda$ for different crystal channels. The calculation was done for 1 GeV positrons using the formula for the dechannelling length from [16, 30]. As one sees from the figure, $\kappa \sim 1$ corresponds to $h\omega = 100–300$ keV for (1 0 0) and (1 1 0) planes in diamond and (1 0 0) plane in silicon. So these channels are the most suitable candidates for using in CUL. This is, however, not the case for a number of other crystals e.g. for graphite and tungsten having $\kappa \gtrsim 10$ in the same photon energy range.

5 X-rays with photon energies of a few tens of keV or less are strongly absorbed in the crystal. This puts the lower limit on the energies of the photons that can be generated by crystalline undulator based devices.

6 Note that $\kappa$ depends weakly (logarithmically) on the particle energy. Therefore, changing the beam energy by an order of magnitude would leave figure 4 practically unchanged.
At $\hbar \omega \sim 10$ MeV, $\kappa$ becomes larger than 10 for all crystal channels. This puts the upper limit on the energies of the photons that can be generated by CUL. It is expected to be most successful in the hundred keV range, while generating MeV photons looks more challenging.

According to our estimations, a brilliance as high as $10^{25} - 10^{26}$ photons/(s mm$^2$ mrad$^2$ 0.1% BW) can be obtained in a CUL fed by a completely modulated positron beam with current 1 kA and particle density $10^{18}$ cm$^{-3}$.

One may expect that the demodulation is not limited to the processes illustrated in figure 2. An additional contribution can come from the energy spread of the channelling particles, as usually happens in ordinary FELs. In fact, the contribution of the energy spread to the beam demodulation on the distance of a few dechannelling lengths is negligible. It would be substantial if the relative spread $\delta E/E$ is smaller than the ratio $\lambda_0/L_d$. The latter ratio, however, cannot be made smaller than $10^{-2}$ [16].

The stochastic energy losses of the channelling particles due to the interaction with the crystal constituents and the radiation of photons. It was shown in [31] that at initial energies of $\sim 1$ GeV or smaller, the average relative energy losses of a positron in the crystalline undulator $\Delta E/E$ are smaller than $10^{-2}$. Clearly, the induced energy spread $\delta E/E \ll \Delta E/E$ is safely below the ratio $\lambda_0/L_d$. From these reasons, we ignored the energy spread of the particles in our calculations.

In conclusion, we have studied the propagation of a modulated positron beam in a bent planar crystal channel. It has been demonstrated that one can find the crystal channels in which the beam preserves its modulation at penetration depths sufficient for producing coherent radiation with a photon energy of hundreds of keV. This opens the prospect for creating intense monochromatic radiation sources in a frequency range which is unattainable for conventional FEL. Developing suitable methods of beam modulation would be the next milestone on the way towards this goal.

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7 Note that the corresponding quantity in ordinary ultraviolet and soft x-ray FELs, the inverse number of undulator periods $1/N_s = \lambda_0/L_d$, is usually of the order of $10^{-3} - 10^{-4}$ [29]. That is why these FELs are so demanding to the small energy spread of the electron beam.