RAY TRACING CALCULATION OF PXR PRODUCED IN CURVED AND FLAT CRYSTALS BY ELECTRON BEAMS WITH LARGE EMITTANCE

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The properties of the parametric X-ray radiation (PXR) produced by beams of relativistic particles passing through flat and bent crystallographic planes have been studied by ray tracing the particles of the incident beam using the well known results on PXR and taking into account multiple scattering. Such calculations are necessary when the electron beam has significant cross section and/or angular spread. As the results of Monte Carlo simulations show in some cases the curved radiators have the advantage that in arrangements like Rowland circles the radiation intensity is much higher than in the case of flat radiators due to PXR focusing. Corresponding experiments are proposed which will confirm the usefulness of microtron and laser produced electron beams for production of monochromatic X-ray beams.

1. Introduction

When a charged particle passes a single crystal under an angle ψ with respect to the crystallographic planes some of pseudophotons accompanying the particle and having frequency $\omega_B = 2\pi c / \lambda_B = \pi c / 2\sin\theta_B$ and the angle $\psi = \theta_B$ satisfying the Bragg condition $2a\sin\theta_B = n\lambda_B$ (n = 1,2…, further we shall consider only the first harmonic, n = 1) will be diffracted and radiated as real photons of a type of radiation which is now called PXR (see [1-5]). Here d is the distance between the crystallographic planes, $\vec{\tau} = \tau\hat{\tau} = 2\pi\hat{\tau} / d$ is the reciprocal lattice vector with unit vector $\hat{\tau}$.

One can interpret PXR also as quasi-Cherenkov radiation, which arises because at certain circumstances the refractive index, which is usually less than one in the x-ray region (see [2]), becomes larger than one in the dynamical theory of x-ray diffraction. Another approach is the PXR interpretation as polarization radiation when the periodically located crystal atoms radiate as in the case of transition radiation (TR) at boundaries between two media. Just as in case of Cherenkov radiation a relation between the PXR emission angle θ (θ is the difference between the radiation and specular directions), ω and particle Lorentz factor γ can be found classically by Huygens construction requiring the difference between the distances from the point spherical sources to observer to be equal to integer number of wavelength.

For the first time PXR as a particular case of coherent radiation produced in three dimensional periodic medium was theoretically investigated in 1969 in the Russian publication of the monograph [1] using the perturbation theory of the classical electrodynamics. Then the theory of PXR was developed by many authors calling it "dynamic radiation" or "quasi-Cherenkov radiation" [2], "parametric X-ray radiation" [4,5], "transition diffracted radiation", "polarization radiation", "Bragg resonant transition radiation", "diffracted X-ray radiation", etc, without remembering that the first author [3] later called this radiation as "X-ray diffraction radiation" (see also [5]). PXR was first experimentally observed in the work [6] with the help of 600 and 900 MeV electrons. To our knowledge at present there are two permanent PXR sources based on 100 MeV [7] and 56 MeV [8] electron linacs.

In all the experiments carried out up today using mainly electrons with energies from a few MeV up to a few GeV the particle beams had small emittance, i.e. small cross section and/or angular spread. However, there are some types of accelerators, betatrons, microtrons etc, which have particle beams with sufficient energies for PXR production but significant emittance. Even using simple pseudophoton interpretation of PXR one can show that the beam with angular spread $\Delta\theta_B$ will result in an expansion of the PXR spectrum, $\Delta\lambda_B / \lambda_B = \Delta\theta_B \cot\theta_B$, and will increase of PXR spot size, decreasing the photon density in them. However, when the electron beam has significant emittance, one may expect that as in the case of X-ray diffraction, the use of bent or curved radiators and Rowland circles can result in a significant increase of the PXR photon density. Bent crystal monochromators have found wide application in synchrotron radiation facilities [9]. In the standard Johann geometry a cylindrically bent crystal provides focusing only for the meridianal rays parallel to the diffraction plane, while the sagittal rays which are oblique to the scattering plane are not focused unless spherically or toroidally bent crystals are not used.

It is worthy to remind that in some publications [10,11] it has been considered the possibility of focusing of PXR produced by particles channeled along the crystallographic planes of bent crystals without any X-ray optics. One can not apply the method of PXR focusing [10,11] when the emittance of the electron beam is relatively large and the particle energies are low.

Of course, it is necessary to develop a correct theory of PXR production in bent crystals as it was done for the theory of Bragg diffraction in bent crystals using or without using accurate Tagaki-Taupin like equations (see, for instance, [12-15] and references therein). Postponing the development of such theories for the future, as a first approximation in this work we shall consider for the first time the production of PXR in curved radiators using the ray tracing methods (see, [15]) developed for X-ray diffraction in flat and bent radiators. As first application of curved radiator for PXR production our consideration is limited only by focusing in scattering plane using radiators with 1D curvature in Johann Rowland circles. Our main assumption, as in [12,15], is: in the points, through which the particles pass, the radiator is taken as flat. We show that the focusing properties of the bent radiator PXR produced by electron beams with significant emittance results in an increase of the PXR photon density. We discuss an experiment which will show the possibility of production of monochromatic, relatively long and femtosecond x-ray pulses with the help of microtron and laser-driven femtosecond electron beams, respectively.

2. Simulation of PXR produced in bent crystals

In the beginning with the help of qualitative considerations let us show that in some simple cases one must expect an increase of PXR density. Indeed, let us consider (see Fig.1) the situation when the radiator has 1D curvature equal to 2*R*, and the electron beam has a significant angular spread. Due to Liouville theoreme with the help of quadrupole lenses Q the beam can be in the scattering plane brought into very small focus (more correctly into a line in the scattering plane) at the "source" plane S of a Rowland circle having curvature radius *R*. Let at the focal plane the electron beam has a Gaussian angular distribution around the direction of the central velocity $\vec{v}$ (see, Fig. 1) of the beam electrons with dispersion $\sigma(\theta_e)$. Let the electrons have sufficiently high energies so that $\sigma(\theta_e) > 1/\gamma$, i.e. the PXR production angles as well as pseudophoton angles are smaller than $\sigma(\theta_e)$. In the case of a symmetric crystal with curvature radius 2*R* by tuning the angle θ_B for the central electrons and neglecting the aberrations, according to the property of the Rowland circle all the PXR photons produced under various angles in Bragg geometry will be refocused in the point (line) F in the "image" or detector plane of the Rowland circle. However, if for the same electron beam one uses flat ($R = \infty$) the point (line) image will be smeared due to absence of focusing. The image of the source at F is larger than in the case of curved crystal. This is an advantage of using curved crystals allowing the increase of the density of PXR photons.

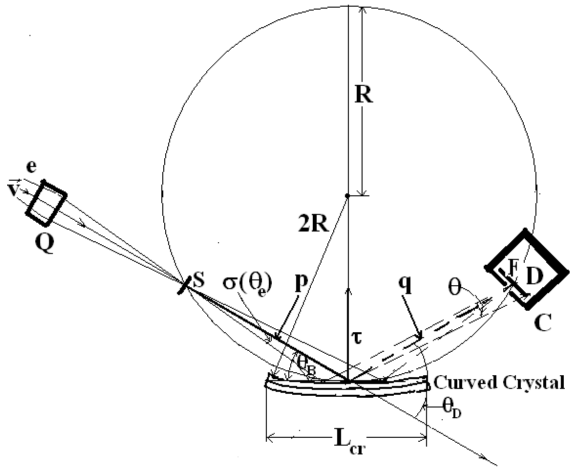


Figure 1. The experimental arrangement. Q is magnetic quadrupole, C is collimator and shielding of the detector D (see the text).

In the general case when the electron beam emittance is not sufficiently small at the plane S and has an “source” spot size, S_e, using the theoretical properties of PXR and making ray tracing of each electrons and produced PXR photons, one can obtain the “image” of the PXR photons on the detector at F with size S_{PXR}. In principle, one can determine the magnification determined as S_{PXR}/S_e. (Point-to-point focusing could be obtained in certain cases of 2D curvature of the crystal, however, here we consider only the simple case of 1D curvature).

According to the kinematical approximation of PXR theory (the more general dynamical and quantum mechanical theories of PXR give no essential corrections, see [16]) one can write the spectral-angular and after integration over photon energy the angular distributions of the number of photons *N* of all polarizations per unit length of crystal in the following forms.

$$\frac{d^2N}{d(\hbar\omega)d\Omega} = \frac{\alpha\omega^3}{2\pi\varepsilon^{3/2}\hbar c^3\beta}\sum_{\vec{\tau}}|\chi_{\vec{\tau}}|^2\left|\frac{[\hat{k},[\hat{k},(\varepsilon\omega\vec{v}/c-\vec{\tau})]]}{((\vec{k}+\vec{\tau})^2-k^2}\right|^2\delta(\omega-(\vec{k}+\vec{\tau})\vec{v}), \tag{1}$$

$$\frac{dN}{d(\Omega)} = \frac{\alpha\omega^3}{2\pi\varepsilon^{3/2}c^3\beta(1-\sqrt{\varepsilon}\hat{k}\vec{v}/c)}\sum_{\vec{\tau}}|\chi_{\vec{\tau}}|^2\left|\frac{[\hat{k},[\hat{k},(\varepsilon\omega\vec{v}/c-\vec{\tau})]]}{((\vec{k}+\vec{\tau})^2-k^2}\right|^2, \tag{2}$$

where $\alpha = e^2/\hbar c = 1/137$ is the fine structure constant,

$$\hbar\omega = \frac{\hbar c\vec{\tau}\vec{v}}{c - \vec{v}\hat{k}} = \frac{2\pi\hbar c}{d}\frac{\beta\sin\theta_B}{1-\sqrt{\varepsilon}\beta\cos\theta}, \quad (3)$$

is the photon energy emitted under polar angle θ with respect to the specular direction with wave vector $\vec{k}$ in the direction with unit vector $\hat{k}$,

$$\chi_{\vec{\tau}}(\omega_B) = S(\vec{\tau})\exp(-W)\frac{\omega_p f(\vec{\tau})}{\omega_B Z}, \quad (4)$$

is the coefficient of the Fourier expansion of susceptibility, $S(\vec{\tau})$ is the structure function; $f(\vec{\tau})$ is the atomic scattering factor, $\exp(-W)$ is the Debye-Waller factor, ω_p is the plasma frequency and Z is periodic number of the crystal material.

The distances *p* and *q* (see Fig.1) between the intersection points S and F on the Rowland circle and central point O on the curved, symmetrically cut crystal is given by

$$p = q = 2R\sin\theta_B. \quad (5)$$

For the general case, when the electron beam has a cylindrical symmetry at the "source" plane with Gaussian distributions radial, $\sigma(r)$, and angular, $\sigma(\theta_e)$, dispersions, with the help of the above given formulae and for the given parameters of the arrangement after dividing the radiator thickness into appropriate number of thin layers to take into account the muyltiple scattering and energy losses, one can carry out the Monte-Carlo simulations procedure of PXR production by ray tracing each of electrons in the following way [17]:

1. Determine the particle parameters on the surface of the crystal-radiator by generating random magnitudes from the distributions describing the beam.
2. Determine the coordinates on the detector and direction of the PXR photon.
3. Determine the deviation of the one of the reciprocal vectors from its average direction.
4. Calculate the characteristics of the PXR photon.
5. With the help of the multiple scattering theory find the particle direction in the next layer.
6. Determine the particle energy taking into account the energy losses.
7. Repeat all this procedures until the particle comes out from the radiator or losses all its energy.

3. Results of calculations

In order to begin the experimental study of the properties of PXR produced in bent crystals we show part of our results carried out for the first time for electron energy 20 MeV, for Si crystal placed in a Rowland circle arrangement (see Fig. 1) with $R = 50$ cm. The chosen angle between the central electrons an the (111) planes of symmetrically cut crystal, $\theta_B = 14.41^\circ$, determines the PXR photon energies $\hbar\omega_B \approx 7.9$ keV and the distances $p = q = 25$ cm. The thickness of the crystal is taken equal to L = 100 μm. As it will be discussed two types of detectors with small and large surfaces can be used for detection of PXR at the image plane F. To make the reasonability and advantages of using of bent crystals more transparent we have calculated the expected properties of PXR for flat and bent crystals for 4 types of electron beams with $\sigma(r)$ and $\sigma(\theta_e)$ at the source plane S described in table 1.

Table 1. Types of the electron beams for which the calculations have been carried out.

NN	Electron Beam	Crystal	$\sigma(r)$ (mm)	$\sigma(\theta_e)$ (rad)
1	Ideal Beam	Flat Bent	0 0	0.0008 0.0008
2	0 cross section, diverging	Flat Bent	0 0	0.008 0.008
3	Thick Pencil	Flat Bent	2 2	0 0
4	General case	Flat Bent	2 2	0.008 0.008

The “ideal beams” of the type 1 are good approximation for almost all the high energy electron PXR experiments carried out up today, while the characteristics of the type 4 are usual for beams from microtrons (see the table in [18]). The small angular divergence 0.0008 rad in the case 1 is taken in order to avoid not desired zeros. The results for the beam types 2 and 3 are given for pedagogical purposes to make the results more transparent.

Fig.2 shows the angular distribution of PXR intensity for an ideal beam (type 1) with flat and curved crystal, respectively. The $\langle\theta_x\rangle$ and $\langle\theta_y\rangle$ - dependences are calculated respectively for fixed θ_x and θ_y equal to $1/\gamma$ when one has peak (maximal) intensity. As expected there is no difference between the results with flat and curved crystals.

Figs.3, 4 and 5 are the same as in Fig. 2 for electron beams of the types 2, 3 and 4, respectively.

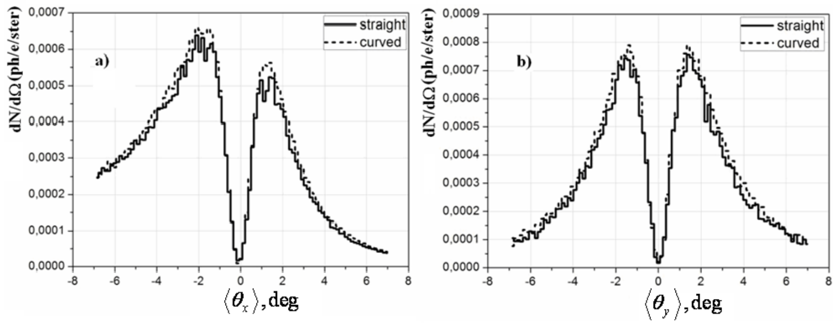


Figure 2. The PXR angular distribution of peak intensity produced in flat a) and curved b) Si crystals (see the text) by an ideal electron beam.

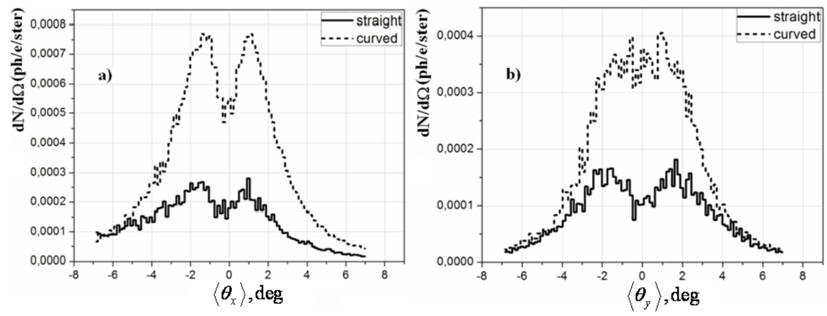


Figure 3. Are the same as in Fig. 2 for electron beam with 0 cross section and finite angular spread (see table 1).

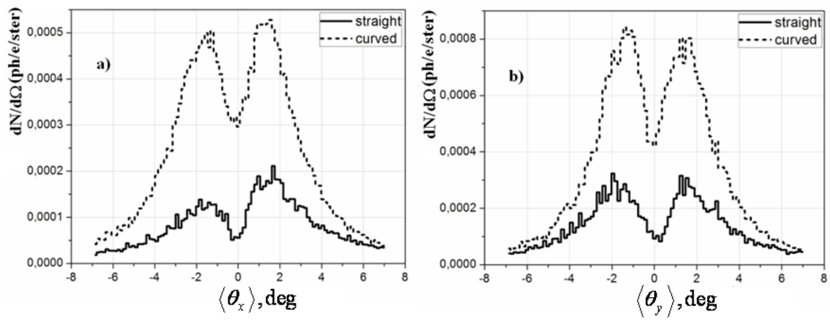


Figure 4. Are the same as in Fig. 2 for "thick pencil" electron beam (see table 1).

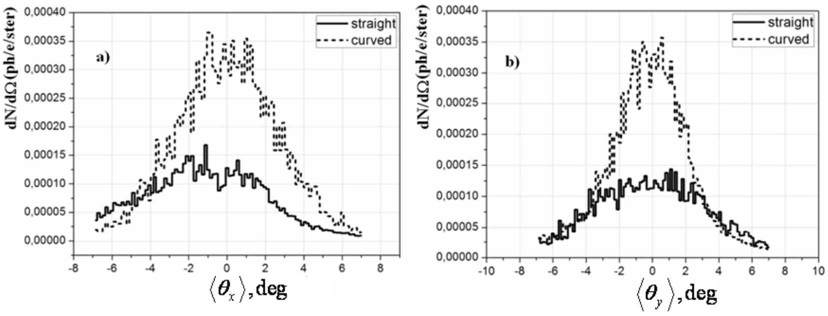


Fig.5. Are the same as in Fig. 2 for electron beam in general case (see table 1).

As it is seen there is an increase in intensity of the angular distributions or of PXR angular density when one uses curved crystal radiator instead of flat one. From the point of experimental results it is important that such an increase exists also for the general case beams from microtrons.

The corresponding PXR spectral distributions measured at angles where the corresponding angular distributions have maximum for flat (solid curves) and curved (dashed curves) crystals which can be measured with the help of small detectors are shown in Fig. 6 a, b, c and d, respectively.

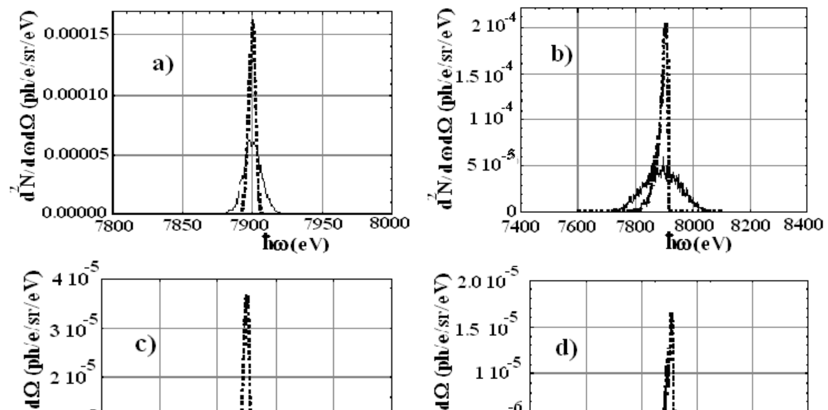
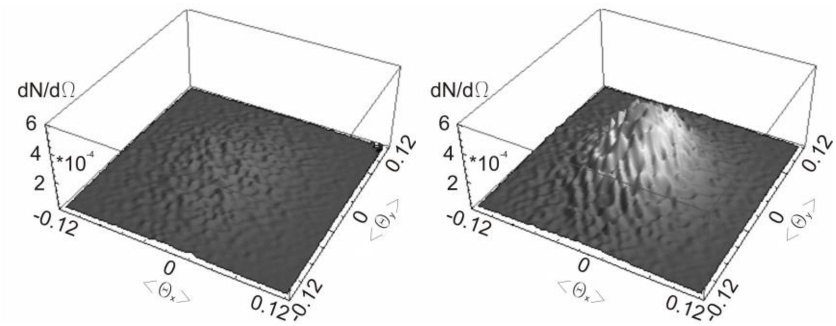


Figure 6. The PXR spectral lines for the cases a) “ideal beam”; b) “0 cross section diverging”; c) “thick pencil” and d) “general case” (see table 1) measured by small surface detector.

The comparison of the results shown in Fig. 6 a, b, c, d, shows that there is an evident narrowing of PXR spectral distributions in the cases of bent crystals compared with the cases of flat crystal.

Finally, in Fig. 7 a and b it is shown the PXR photon density angular distributions for flat a) and curved crystals which can be measured by a large acceptance detector. The curves of the Fig. 2-5 are the corresponding cross sections of the 3D PXR intensity angular distributions.



(a) (b)

Figure 7. The 3D angular density distributions of PXR produced by electron beam of general case 4) in flat a) and curved b) crystals measured by a large surface detector.

4. Experimental Considerations

As it has been mentioned above all the PXR experiments were carried in the assumption of “ideal beam” using electron beams from linacs or high energy cyclic accelerators with small angular spread. No Rowland circles were used, which besides the X-ray diffraction experiments, in our knowledge, was successfully used only in the work [19] to focus the isotropic characteristic radiation. However, the electron beams of low energy cyclic accelerators, such as microtrons [18,20] and synchrotrons [21,22] have beam size ~ (2-4) mm^2 and angular spread ~ (1-4) mrad. It is better to reduce the direct background from the accelerator and to change the beam sizes at the point F1 at the entrance of the experimental arrangement with Rowland circle with the help of magnets and quadrupoles as in [18] and it is shown in Fig. 1.

Preliminary it is planned to perform the experiment at YerPhI (10-20) MeV microtron, M-25, where as at [18] after deflection and quadrupoles there is a beam with the parameters:

Table 2. Parameters of the YerPhI microtron M-25 electron beam.

Beam parameter	Value (unit)
Electron energy	(10-25) MeV
Macropulse length	$2\ 10^{-6}$ s
Repetition rate	400 Hz
Micropulse length	$\sim 2\ 10^{-11}$ s
Number of electrons per micropulse	$3\ 10^{7}$
Number of micropulses per macropulse	6000
Electron beam cross section	~ 4x2 mm^2
Emittance (horizontal and vertical)	$3\ 10^{-2}$ and $1.5\ 10^{-2}$ mm rad

Though toroidically and spherically bent crystals providing focusing in 2 dimensions are used in diffraction, synchrotron radiation and neutron physics experiments in this test experiment we assume to use the methods of described in [23] for preparation of cylindrically bent 4x4x0.01 cm^3 Si(111) crystal with curvature radius R = 100 cm.

As in the proposed ring transition radiation detectors [24] two types of large acceptance position sensitive and small spectrometric detectors can be used for detection of PXR photons with energies 6-12 keV. As first type detector a 2 cm thick MPC with 50 micron thick mylar window and filled with xenon can provide ~ 10% energy and ~ 100 micron space resolutions, while a CCD array with special coating (as in X-ray cameras available from Hamamatsu and other companies) can provide ~ 30% energy and a few tens microns space resolutions during the large acceptance measurements. Taking into account all the processes the efficiencies of these detectors are approximated by polynomials [24]

$$\varepsilon_{MPC} = 0.0009(\hbar\omega)^3 - 0.0381(\hbar\omega)^2 + 0.4262(\hbar\omega) - 0.5087\,, \qquad (6)$$

$$\varepsilon_{CCD} = 0.0042(\hbar\omega)^3 - 0.0972(\hbar\omega)^2 + 0.6121(\hbar\omega) - 0.2281\,, \qquad (7)$$

in which the photon energies are measured in keV. As a second type of detector a 2.5x2.5 mm^2 solid state X-100 Amptek Inc. detector will provide much better than ~ 150 eV energy resolution during low acceptance angular and spectral measurements.

Taking into account the electron beam intensity (see table 2), the angular acceptances of the detectors and the above given results of the Fig. 2-6, it will be required a few hours pure measurement times for obtaining one angular and spectral curve (of the types given in Fig. 2-6) consisting of 10 points with mean 10% statistical errors or for obtaining one wide acceptance angular distribution (as in Fig. 7).

5. Conclusions

In this work for the first time it has been studied the PXR produced by particle beams with significant emittance in flat and curved crystals. It has been proposed an experiment which can be performed on microtrons and in which using Rowland circle arrangement one can increase the PXR density compared with the case of flat crystals.

The validity of the main assumption, namely, that at the points, through which the particles pass, one can consider the curved radiator as flat, can be justified by the facts that usually the transversal formation sizes of the radiation is of the order of $\sim \lambda\gamma$ which is small and by the correct results obtained by simulation of X-ray diffraction based on the same assumption. The generalization of concave (menisc) and 2D (eliptical) curvature cases and Laue geometry is trivial as it follows from the works devoted to X-ray diffraction monochromators. The proposed method based on the properties of Rowland circle can be used also for calculating the PXR production in flat and curved gradient crystals and multilayers as well as for other types of radiation as transition radiation produced in curved radiators.

At present intense femtosecond electron beams with energies up to a few GeV are produced on table top arrangements with the help of laser beam [25]. However, the emittance of the laser produced electron beams is worse than that of the linac beams, and improvement works are necessary before they use for production X-ray beams by SASE mechanism, though their possibility for undulator [26] and inverse Compton [27] X-ray beam production has been proven. The X-ray pulses produced with the help of these laser driven electron beams by PXR mechanism will be not only femtosecond, but more monochromatic that the ones by the methods [26, 27].

The main conclusion is: The already existing low energy microtrons which give more intense electron beams than the linacs, as well as the laser produced femtosecond electron beams with slightly worse emittance can be used for production of monochromatic X-ray beams by PXR mechanism.

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