FIRST ORDER PERTURBATION THEORY EVALUATION OF INITIAL STAGE OF SELF AMPLIFIED CRYSTAL-BASED X-RAY EMISSION

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Abstract

Mechanisms of x-ray generation by relativistic electrons in the energy range below 100 MeV by interaction with crystals are discussed in view of possibility to obtain self amplification of spontaneous emission. To investigate the initial stage of self amplified spontaneous emission process the first-order perturbation theory that enables to describe the collective beam response as effective susceptibility is used. Based on this approach Cherenkov radiation in the anomalous dispersion frequency range, parametric x-ray radiation and axial channeling radiation mechanisms are considered. The axial channeling mechanism in the case of grazing incidence electrons was shown to be most promising one.

INTRODUCTION

X-ray Free Electron Lasers (XFELs) open new revolutionary opportunities for investigations in materials science, chemistry, biology and other areas. However, due to high cost of construction and maintain, the access to these facilities for wide scientific community is quite limited. This motivates search for schemes of compact bright x-ray sources. The size of X-ray Free Electron Lasers is dictated by basic properties of undulator radiation: to produce x-rays with Angstrom wavelength from cm period undulator one needs electrons with energy in GeV range. If one considers the radiation mechanisms accompanying the propagation of electron beam through a crystal structure (channeling radiation, parametric x-ray radiation, Cherenkov radiation near K-edge), one can see that to get photons in x-ray range one needs electrons with energy of tens to hundreds MeV. The dramatic 10 orders of magnitude increase of brightness of XFELs compared to III generation synchrotron became possible due to phenomenon of self amplified spontaneous emission (SASE). In the case of XFELs the spontaneous emission which is amplified is the undulator radiation, the SASE process being developed due to high charge, short duration and small emittance of the bunch as well as long undulator length. In the present paper we will investigate the possibility of SASE process for which as a spontaneous radiation mechanisms serve x-ray radiation mechanisms in crystals. The development of rigorous SASE theory in this case is extremely difficult task due to large number of phenomena accompanying electron propagation in crystals and complexity of SASE phenomena itself, however, one can use the first order perturbation theory to describe the first stage of SASE process [1] and determine the most promising radiation mechanism and experiment geometry.

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RADIATION MECHANISMS

One of the ways to find at which conditions x-ray radiation of electrons in crystal will take place is to find phase match between the electromagnetic field that can exist in the crystal and current of electron in the crystal. In the Fourier space this condition can be expressed as intersection of dispersion surface of electromagnetic radiation

$$k^2 - \frac{\omega^2}{c^2}(1+\chi(\omega)) = 0 \tag{1}$$

here $\chi(\omega)$ is the susceptibility of the crystal; and condition that should be satisfied for Fourier components of a single electron current

$$\omega - \vec{k}\cdot\vec{v} = 0 \tag{2}$$

here $\vec{v}$ is the velocity of electron. In order to organize intersection of (1) and (2) one can act in two ways: either modify properties of the medium to bring (1) in intersection with (2), or modify the movement of the electron and correspondingly (2) to bring it in intersection with (1). Let us name the first scenario as case I and the second as case II.

In the x-ray domain for electrons in crystals case I can be realized if $\mathrm{Re}\chi(\omega) > 0$ that leads to Cherenkov radiation, or under the Bragg diffraction conditions under which dispersion equation (1) is modified to

$$\left[k^2 - \frac{\omega^2}{c^2}(1+\chi_0)\right]\left[(\vec{k}+\vec{H})^2 - \frac{\omega^2}{c^2}(1+\chi_0)\right] - \chi_{\vec{H}}\chi_{-\vec{H}}\frac{\omega^4}{c^4} = 0 \tag{3}$$

here $\vec{H}$ is the reciprocal lattice vector for which the Bragg condition $(\vec{k}+\vec{H})^2 = k^2$ is satisfied, $\chi_{\vec{H}}$ is the spatially periodic part of the susceptibility corresponding to crystallographic planes with reciprocal lattice vector $\vec{H}$, the polarization in the plane orthogonal to vectors $\vec{k}$, $\vec{H}$ is considered for simplicity. Under the conditions of intersection of (3) with (2) parametric x-ray radiation takes place.

The case II can be realized if one introduce oscillatory component in the electron current. In the case of relativistic electrons in the crystal, the oscillatory component can appear if the electron goes into the channeling regime, in this case (2) is modified to

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$$\omega - \vec{k}\cdot\vec{v} - \omega_{if} = 0, \quad (4)$$

here ω_{if} is the frequency of transition between initial and final states of transverse channeling motion. Under the conditions of intersection between (4) and (1) the channeling radiation takes place.

SASE ESTIMATIONS FOR CHERENKOV AND PARAMETRIC X-RAY RADIATION

The SASE effect is conditioned by action of radiated electromagnetic field on the electrons and back action of the induced current on the electromagnetic field. In the frame of first order perturbation theory this process leads to component of the beam current that is proportional to the acting electromagnetic field, hence in terms of interaction with electromagnetic field the presence of the beam can be described as an active medium. Based on the Vlasov equation one can show that the induced susceptibility tensor is

$$\chi_b(\vec{k},\omega) = -\frac{4\pi e^2}{m_e\gamma\omega^2}\int d^3\vec{p}f^{(0)}(\vec{p})[1 + \frac{\vec{v}\otimes\vec{k}+\vec{k}\otimes\vec{v}}{\omega-\vec{k}\cdot\vec{v}} + k^2\frac{\vec{v}\otimes\vec{v}}{(\omega-\vec{k}\cdot\vec{v})^2}] \quad (5)$$

here $f^{(0)}(\vec{p})$ is initial distribution of electron momenta in the beam, the sign $\otimes$ denoted the diad (Kronecker) product.

Cherenkov radiation

In the x-ray frequency domain the susceptibilty of a crystal is negative and is mainly determined by total electron density. However, near frequencies corresponding to transitions from inner electron shells, e.g. K-edges, the corresponding electronic transitions give significant contribution to susceptility and in the harrow range the susceptibility can become positive. Inevitably, in the same region the imaginary part of the susceptibility responsible for absorption increases as well.

Consider a frequency at which the crystal susceptibility is positive that leads to Cherenkov radiation. The analysis of SASE possibility can be performed by means of considering the dispersion equation of electromagnetic field in the medium and active medium described by (5). The wave equation for electromagnetic field in such a medium reads

$$L(\vec{k},\omega)\cdot\vec{E}(\vec{k},\omega) = 0, \quad (6)$$
$$L(\vec{k},\omega) = k^2 - \vec{k}\otimes\vec{k} - \frac{\omega^2}{c^2}(1+\chi_0+\chi_b(\vec{k},\omega))$$

here scalar quantities entering in L are assumed to be multiplied by a unit matrix. The dispersion equation is obtained from condition $DetL = 0$. If one considers normal incidence and solve the dispersion equation in terms of deviation of the wavevector δk_z from the resonance conditions at which intersection of (1) and (2) takes place, one arrives at

$$\left(2\frac{\delta k_z}{\omega} - i\chi''\right)\frac{\delta k_z}{\omega}^2 \simeq \frac{\omega_b^2}{\gamma\omega^2}4\chi_0^2 \quad (7)$$

here one has taken into account that the beam plasma frequency is much smaller than x-ray frequency, beam emittance was considered to be infinitely small, the exact resonance conditions are fulfilled, χ'' is imaginary part of the susceptibility. If one considers very optimistic parameter for the focused electron bunch current density $j \sim 10^{10}A/cm^2$ and neglect χ'' in (7), for typical x-ray frequency of 10keV one obtains Im$\frac{\delta k_z}{\omega} \sim 10^{-6}$. This value is about 3 orders of magnitude less than imaginary part of the susceptibility responsible for absorption, hence Cherenkov based SASE process in x-ray domain hardly can be expected.

Parametric x-ray radiation

In the case of parametric x-ray radiation the equation analogous to (6) takes the form

$$[k^2 - \vec{k}\otimes\vec{k} - \frac{\omega^2}{c^2}(1+\chi_0)]\vec{E}_0(\vec{k},\omega) \quad (8)$$
$$-\frac{\omega^2}{c^2}\chi_{-\vec{H}}\vec{E}_H(\vec{k},\omega) = \frac{\omega^2}{c^2}\chi_b(\vec{k},\omega)\vec{E}_0(\vec{k},\omega)$$
$$[(\vec{k}+\vec{H})^2 - (\vec{k}+\vec{H})\otimes(\vec{k}+\vec{H}) -$$
$$\frac{\omega^2}{c^2}(1+\chi_0)]\vec{E}_H(\vec{k},\omega) - \frac{\omega^2}{c^2}\chi_{\vec{H}}\vec{E}_0(\vec{k},\omega) = 0$$

here $\vec{E}_H(\vec{k},\omega)$ corresponds to Bragg-diffracted wave. A detailed analysis of (8), calculation of dispersion equation, evaluation of emittance effect and analysis of SASE process based on boundary conditions can be found in [2]. The analysis shows that for optimized geometry of $\vec{k},\vec{v},\vec{H}$ direction, and under the most favorable conditions and value for the bunch current $j \sim 10^{10}A/cm^2$ one arrives at intensity e-folding crystal thickness of about 1 mm. After such distance in the crystal the beam would suffer drastic multiple scattering that would degrade the induced susceptibility due to the integration in (5). This would degrade the SASE process, hence the parametric x-ray radiation SASE scenarion has significant difficulties as well.

SASE ESTIMATIONS FOR CHANNELING RADIATION

The process of multiple scattering can be significantly changed if electrons of the beam are under conditions of channeling. In this case electrons are trapped by potential of atomic plane or atomic string, the transverse motion being described by Schrodinger equation with effective mass γm. If one is interested in x-ray radiation wavelength in the Angstrom range, the corresponding electron energy is below 100 MeV, in this energy range the quantum description

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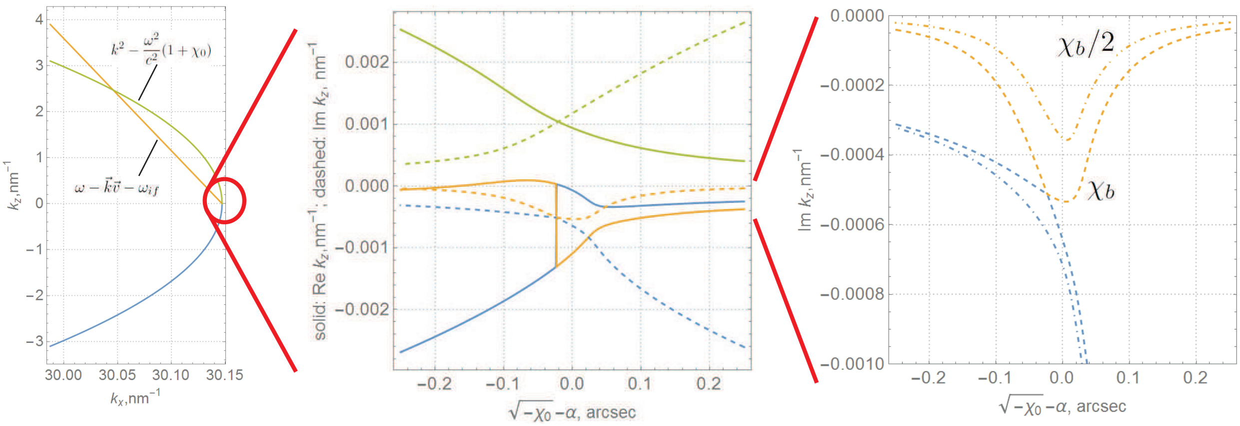

Figure 1: Dispersion surface under the grazing incidence conditions, magnified from left to right under. Parameters used: electron energy 25 MeV, bunch charge 1 nC, bunch length 0.1 ps, emittence is $\epsilon_n = 0.1$mm$\cdot$mrad, LiH crystal, channeling direction $< 110 >$, corresponding x-ray energy is 5.9 keV.

of electron channeling is essential. The action of electromagnetic field on channeled electrons and back within the first order quantum mechanical perturbation theory can be described by induced susceptibility as well as in the case I, the corresponding expression reads:

$$\chi^{(b)}(\vec{k},\omega) = \chi_b \frac{\omega\vec{\zeta}\otimes\vec{\zeta}}{\omega - \vec{k}\vec{v} - \omega_{if}}, \qquad (9)$$

$$\chi_b = \frac{4\pi n_e e^2}{\omega^3}(P_i - P_f)\omega_{if}^2 m_{if}^2,$$

$$\vec{\zeta} = \vec{n}_c + \vec{v}\frac{\vec{k}\vec{n}_c}{\omega_{if}},\ m_{if}\vec{n}_c = \langle\phi_i|\,\vec{r}_\perp|\phi_f\rangle$$

here axial channeling is assumed, $\vec{n}_c$ is the crystallographic direction along which channeling is taking place, $|\phi_i\rangle, |\phi_f\rangle$ are wavefunctions of initial and final states, P_i, P_f are occupations of these states. In contrast to the case I, in order to describe the spontaneous emission of channeling radiation one has to treat the noise current of channeled particles quantum-mechanically:

$$\hat{\vec{j}}_0(\vec{k},\omega) = -ie\sum_i \hat{\sigma}_-^{(i)} e^{-i\vec{k}\vec{r}_i^{(0)}} m_{if} \times \qquad (10)$$

$$\omega_{if}\vec{\zeta}\delta(\omega - \vec{k}\cdot\vec{v} - \omega_{if}) + h.c.,\ \hat{\sigma}_- = |i\rangle\langle f|$$

The electromagnetic field operators should be treated quantum mechanically as well, however if we use the Heisenberg picture one can apply boundary conditions similar to the classical case and use form similar to Maxwell equations to calculate observable values [3]. The electromagnetic field in the crystal can be presented as

$$\hat{\vec{E}}(\vec{k},\omega) = \sum_s \hat{\vec{E}}_s(\vec{k}_{||},\omega)\delta(k_z - k_z^{(s)}(\vec{k}_{||},\omega)) + \qquad (11)$$

$$G(\vec{k},\omega)\frac{4\pi i\omega}{c}\hat{\vec{j}}_0(\vec{k},\omega)$$

here the first summand corresponds to homogeneous part of the electromagnetic field that is described based on equation similar to (6) with susceptibility (9) instead of (5), $k_z^{(s)}$ are the solutions of the dispersion equation Det$L(\vec{k},\omega) = 0$ as a function of frequency ω and component of the wavevector parallel to the crystal surface $\vec{k}_{||}$; the second summand corresponds to inhomogeneous part of the field due to spontaneous current, $G(\vec{k},\omega) = L(\vec{k},\omega)^{-1}$ is the Green function.

In the considered case at the intersection of (4) and (1) that corresponds to direction given by deviation from surface normal equal to $\theta = \sqrt{2\omega_{if}/\omega - 1/\gamma^2 - |\chi_0|}$, the imaginary part of the wavevector comes out to be $\delta k = \pm i\frac{\omega}{c}\sqrt{\frac{\chi_b}{2}}$ that under the conditions given at Fig.1 results in gain length about 0.8 mm that is much larger than the dechanneling length.

However, this length can become significantly smaller if larger number of dispersion surface branches are brought to resonance. This situation can take place if the dispersion surface (4) comes close to the dispersion branches corresponding to transmitted and reflected waves, see Fig.1. In this case if channeling axes makes angle $\alpha = \sqrt{|\chi_0|}$ to the sample surface and the radiation is observed at angle $\beta = \sqrt{2\omega_{if}/\omega - 1/\gamma^2 - |\chi_0|}$ one can obtain based on the dispersion equation for deviation from resonance that $\delta k_z = \pm i\frac{\sqrt{3}}{2}\frac{\omega}{c}\left(\frac{\chi_b}{\beta}\right)^{\frac{1}{3}}$ if the conditions $\left(\frac{\chi_b}{\beta}\right)^{\frac{1}{3}} \sim (\mathrm{Im}\chi_0)^{\frac{1}{2}}$ are fullfilled. In the case of parameters of Fig.1 one can see that the gain length decreases to a quantity comparable with the dechanneling length. In the future work we plan to investigate this case in more details.

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