INITIAL STAGE OF SELF AMPLIFIED RADIATION EMISSION FROM ELECTRON BUNCHES IN CRYSTAL: LINEAR RESPONSE THEORY

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Abstract

Self amplified spontaneous emission (SASE) is a key process in X-ray free electron lasers' operation. In this case the spontaneous emission is undulator radiation emission, the radiation in X-ray range being possible from electrons in GeV energy range. In the case of interaction of electrons with properly aligned crystal the channeling radiation results in X-rays from electrons with energies in tens MeV energy range. In this situation for high current densities the SASE process may take place that potentially could lead to construction of a compact bright X-ray source. In present contribution the first principle theoretical description is outlined and first order perturbation theory is used to model the initial stage of SASE. The transition from spontaneous to SASE regime is described, the requirements for bunch current and emittance are determined. By means of dispersion equation analysis and boundary condition application the intensity radiated from crystal slab is calculated and it is shown that Bragg diffraction could enhance self amplification. A numerical example for Si (001) illustrates the model.

INTRODUCTION

High brightness fs short x-ray pulses are unique tools to investigate structure and dynamics of matter. X-ray beams of this kind are produced at the X-ray Free Electron Laser (XFEL) facilities where electrons accelerated to GeV energy radiate coherently in hundreds meters long undulators. The km large scale of XFELs as well as synchrotrons is conditioned by the basic properties of undulator radiation which is the underlying mechanism of x-ray production. The high overbooking of existing facilities motivates the search for compact sources of bright and short x-ray pulses relying on different mechanisms of x-ray generation and electron acceleration.

The electron energy needed to generate x-rays can be reduced to tens of MeV if one considers x-ray generation due to interaction of electrons with crystalline targets, the generation mechanisms include Cherenkov radiation near K-edge, parametric x-ray radiation, channeling radiation and others. The principal drawback of the sources based on these radiation mechanisms is low number of emitted x-ray quanta which is conditioned by limitations on interaction length and current densities. The brightness of the source increases drastically in situation when electrons radiate coherently. The coherence in radiation between electrons can be achieved in two ways: the electron bunch can be modulated in advance with modulation period equal to radiation wavelength, or the electron beam can become bunched itself due to interaction with the generated radiation resulting in the phenomenon of self amplified spontaneous emission (SASE).

In the present contribution we consider the possibility of SASE process, the spontaneous emission being the channeling radiation. The SASE process requires large current density low emittance electron beams and large interaction lengths. However, the progress in the field of generation of low emittance fs short electron beams makes the needed electron properties close to reality. Also, the "diffraction before destruction" concept which in our case can be reflected as "radiation before destruction" concept lifts restrictions on beam current density in the case of fs short electron bunches. In this paper we use the linear response theory to describe the initial stage of channeling radiation SASE process and find the conditions at which SASE can be observed. In order to favor the conditions for SASE onset and reduce the requirements for the beam we take advantage of the crystallographic order in a way that it forms the distributed feedback, which is known to improve the lasing properties.

The paper is organized as follows: In first section channeling radiation is briefly described and the way how first principle exact description can be build is outlined, next we consider simplified approach within the first order perturbation theory which leads to treatment of the electron beam as an active medium, the intensity being determined from boundary conditions, within this approach the SASE process is described in terms of imaginary part of dispersion equation solution, and finally a numerical example of Si(001) is given.

CHANNELING RADIATION AND FIRST PRINCIPLE FORMALISM

When a relativistic electron enters the crystal in a direction close to a crystallographic axes the channeling phenomena takes place: electron's motion in direction orthogonal to crystallographic axes is bounded and determined by an average potential of the atoms constituting the axes. It can be shown that the transverse motion can be described by a non-relativistic Schrodinger equation with effective mass γm where γ is the relativistic factor, m is electron rest mass. In the electron's energy range of tens of MeV the quantum mechanical treatment is necessary, in contrast to GeV energy range where classical description is sufficient, and one can find transverse energy states and their occupations conditioned by state of the electron at the entrance to the crystal. The oscillations of electron around the crystallographic axes (in classical descriptions) or transition between the transverse energy levels (in quantum description) results in spontaneous channeling radiation. The radiation properties are close to that of undulator radiation, the radiation

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frequency ω being centered at

$$\omega = \frac{2\gamma^2\Omega}{1+\gamma^2\theta^2}, \qquad (1)$$

here Ω is transition frequency between the transverse energy levels, the peak photon density in forward direction being

$$\frac{dN}{d^2\vec{n}d\omega/\omega} = 4\alpha K_u^2 N_u^2 \gamma^2 P_e, \qquad (2)$$

$$K_u = \gamma\frac{\Omega d_{eg}}{c}, \quad N_u = \frac{\omega L}{4\pi\gamma^2},$$

here $\alpha = 1/137$, d_{eg} is dipole moment for the transition between excited and ground channeling states, P_e is the occupation of excited channeling state.

For high current density of channeling electrons one has to consider the evolution of radiation in crystal and state of channeled electrons self-consistently, the feedback of radiation toward electrons leading to SASE process. Considering the transitions between excited $|e\rangle$ and ground $|g\rangle$ channeling states one can derive from the first principles Hamiltonian the Heisenberg equation for operator of electromagnetic field vector-potential $\hat{\vec{A}}(\vec{r},t)$ and operators describing the channeling states $\hat{\sigma}_{eg} = |e\rangle\langle g|$, $\hat{\sigma}_{zz} = |e\rangle\langle e| - |g\rangle\langle g|$:

$$\Delta\hat{\vec{A}}(\vec{r},t) - \frac{\epsilon(\vec{r})}{c^2}\frac{\partial^2\hat{\vec{A}}(\vec{r},t)}{\partial t^2} - \vec{\nabla}(\vec{\nabla}\cdot\hat{\vec{A}}(\vec{r},t)) = \qquad (3)$$

$$\frac{4\pi i}{c}\sum_i e\Omega\hat{\sigma}_{eg}^{(i)}(t)\times$$

$$[\vec{d}_{eg} + \frac{i}{\Omega}\vec{u}(\vec{d}_{eg}\cdot\vec{\nabla})]\delta(\vec{r}-\vec{r}_0^{(i)}-\vec{u}t) + h.c.$$

$$\frac{\partial\hat{\sigma}_{eg}^{(i)}(t)}{\partial t} = i\Omega\hat{\sigma}_{eg}^{(i)}(t) + \hat{\sigma}_{zz}^{(i)}(t)\frac{e\Omega}{\hbar c}\times$$

$$[\vec{d}_{eg} + \frac{i}{\Omega}\vec{u}(\vec{d}_{eg}\cdot\vec{\nabla})]\hat{\vec{A}}(\vec{r},t)|_{\vec{r}=\vec{r}_0^{(i)}+\vec{u}t} + h.c.$$

$$\frac{\partial\hat{\sigma}_{zz}^{(i)}(t)}{\partial t} = \hat{\sigma}_{eg}^{(i)}(t)\frac{2e\Omega}{\hbar c}\times$$

$$[\vec{d}_{eg} + \frac{i}{\Omega}\vec{u}(\vec{d}_{eg}\cdot\vec{\nabla})]\hat{\vec{A}}(\vec{r},t)|_{\vec{r}=\vec{r}_0^{(i)}+\vec{u}t} + h.c.$$

here $\vec{u}$ is electron's velocity along the channeling axes, $\vec{r}_0^{(i)}$ is its initial position, $\epsilon(\vec{r})$ is dielectric permittivity of the crystal.

LINEAR RESPONSE THEORY

The system (3) is difficult to handle since it is formulated for non-commutating operators and has non-linear terms. It can be simplified for the initial stage of SASE process when electromagnetic field vector-potential and the change of occupations can be assumed to be small. In the zeroth approximation if one assumes that $\hat{\sigma}_{eg}(t) = e^{i\Omega t}\hat{\sigma}_{eg}(0)$, $\hat{\sigma}_{zz}(t) = \hat{\sigma}_{zz}(0)$ from (3) one can get the value of radiation field amplitude that will be proportional to $\hat{\sigma}_{eg}(0)$. Performing the quantum-mechanical averaging $\langle\hat{\sigma}_{eg}(0)\rangle = 0$, $\langle\hat{\sigma}_{eg}(0)\hat{\sigma}_{ge}(0)\rangle = P_e$ one obtains the expression for spontaneous channeling radiation.

If one considers the first order perturbation theory one can find from (3) a contribution to $\hat{\sigma}_{eg}(t)$ proportional to electromagnetic field vector-potential, it results in an effective susceptibility due to linear response of the electron beam to electromagnetic field, in Fourier $\vec{k},\omega$ space it takes the form

$$\chi^{(b)}(\vec{k},\omega) = \chi_b\frac{\omega}{\omega - \vec{k}\vec{v} - \Omega}\vec{a}\otimes\vec{a}, \qquad (4)$$

$$\chi_b = \frac{4\pi ecj\Delta P}{\hbar\omega^3}\frac{\Omega^2 d_{eg}^2}{c^2}, \quad \vec{a} = \frac{\vec{d}_{eg}}{d_{eg}} + \vec{v}\frac{\vec{k}\vec{d}_{eg}}{\Omega d_{eg}},$$

here $\Delta P = P_e - P_g$, j is electron beam current density. Within this treatment the equation for electromagnetic field in the crystal (3) in Fourier space results in

$$[X_k I - \vec{k}\otimes\vec{k} - \frac{\omega^2}{c^2}\chi^{(b)}(\vec{k},\omega)]\cdot\vec{A}_k(\vec{k},\omega) - \qquad (5)$$

$$\frac{\omega^2}{c^2}\chi_{-H}\vec{A}_H(\vec{k},\omega) = \frac{4\pi}{c}\vec{j}_{(sp)}(\vec{k},\omega)$$

$$[X_H I - (\vec{k}+\vec{H})\otimes(\vec{k}+\vec{H})]\cdot\vec{A}_H(\vec{k},\omega) -$$

$$\frac{\omega^2}{c^2}\chi_H\vec{A}_k(\vec{k},\omega) = 0,$$

$$X_k = k^2 - \frac{\omega^2}{c^2}(1+\chi_0),$$

$$X_H = (\vec{k}+\vec{H})^2 - \frac{\omega^2}{c^2}(1+\chi_0),$$

here we have taken into account the crystallographic order present in the crystal that results in periodic permittivity $\epsilon(\vec{r}) = 1 + \chi_0 + \chi_H e^{i\vec{h}\vec{r}} + \chi_{-H}e^{-i\vec{h}\vec{r}}$ and assume that the emitted radiation is close to Bragg conditions for reciprocal lattice vector $\vec{H}$ (a two-wave approximation), the current density $\vec{j}_{(sp)}(\vec{k},\omega)$ corresponding to spontaneous radiation appearing within the zeroth order approximation is

$$\vec{j}_{(sp)}(\vec{k},\omega) = \qquad (6)$$

$$2\pi ie\Omega d_{eg}\vec{a}\delta(\omega - \vec{k}\vec{u} - \Omega)\sum_i e^{-i\vec{k}\vec{r}_0^{(i)}}\hat{\sigma}_{eg}^{(i)}(0).$$

From (5) one can find the homogeneous solution of the wave field inside the crystal

$$\vec{A}(\vec{k},\omega) = \sum_s A_s(\vec{k},\omega)\vec{e}_s(\vec{k},\omega)\delta(k_z - k_z^{(s)}(\vec{k}_{||},\omega)) \qquad (7)$$

here index s corresponds to the solutions of the dispersion equation, A_s are the amplitudes to be found from the boundary conditions, $\vec{e}_s$ are the polarization vectors, $k_z^{(s)}(\vec{k}_{||},\omega)$ are the solutions of the dispersion equation. The dispersion equation can be factorized in dispersion equations corresponding to σ and π polarizations in a practically important case when the ground state is double degenerate giving rise to two orthogonal and equal in magnitude values of $\vec{d}_{eg_1}, \vec{d}_{eg_2}$. In this case the expression for σ polarization takes the form

$$[X_k X_H - \frac{\omega^4}{c^4}\chi_H\chi_{-H}](\omega - \vec{k}\vec{u} - \Omega) = \chi_b X_H\frac{\omega^3}{c^2}. \qquad (8)$$

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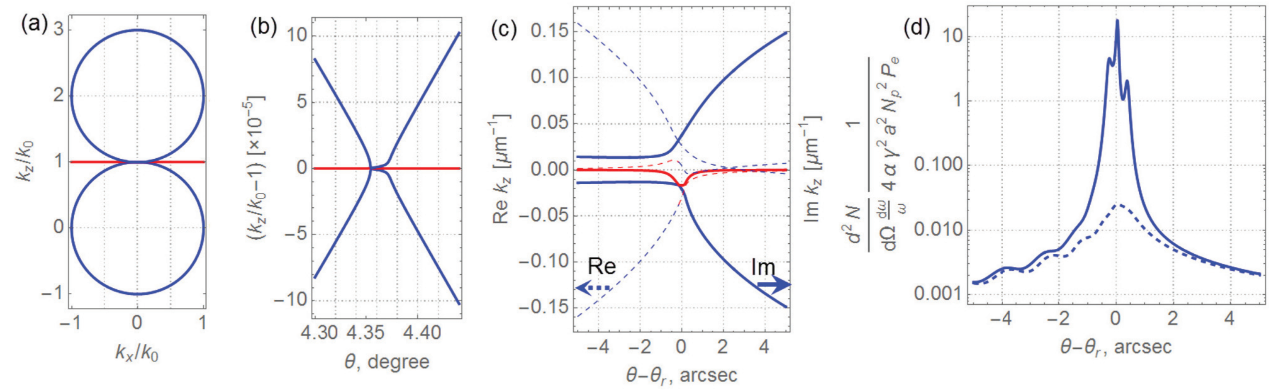

Figure 1: Dispersion surface and channeling radiation intensity, see details in text, a - general view of dispersion surface, b - dispersion surface in the vicinity of Bragg conditions, c - detailed view near the resonance conditions, blue lines - dispersion equation solution corresponding to dynamical diffraction roots, red lines - to channeling radiation condition; d - radiation intensity profile, solid line represents SASE effect, dashed line corresponds to spontaneous radiation.

The amplification of spontaneous radiation takes place at the intersection of dispersion equation $X_k X_H - \frac{\omega^4}{c^4}\chi_H\chi_{-H} = 0$ corresponding to Bragg diffraction and $\omega - \vec{k}\vec{u} - \Omega = 0$ corresponding to channeling radiation condition. At the intersection the right hand side of (8) becomes important for dispersion equation solution and leads to imaginary addend to dispersion equation roots [1]. It corresponds to instability increment and describes the initial stage of SASE process. To determine the amplitudes A_s of the radiation field one has to apply boundary conditions for the field similar to used in dynamical diffraction theory and in addition for the current density, since the number of roots of (8) is larger by one compared to dynamical diffraction case. The corresponding boundary condition (for σ polarization) can be transformed to

$$8\pi^2 ie\Omega d_{eg} \sum_i e^{-i\vec{k}\vec{r}_0^{(i)}} \hat{\sigma}_{eg}^{(i)}(0) = \sum_s A_s \frac{[X_k X_H - \frac{\omega^4}{c^4}\chi_H\chi_{-H}]}{X_H\omega^2/c^2}\Big|_{k_z=k_z^{(s)}}. \tag{9}$$

One can see that far from dispersion roots intersection the main contribution to (9) comes from the root corresponding to channeling radiation and results in similar expressions as for the spontaneous radiation case.

NUMERICAL EXAMPLE FOR Si (001)

Consider the case of axial channeling along [001] direction in Si crystal and the channeling radiation satisfying the Bragg condition for 004 reflexion at Bragg angle close to $\pi/2$, the resulting x-ray photon energy is 4.5 keV. For 25 MeV electrons moving along channeling axis the occupation of the energy levels calculated within the Moliere potential show population inversion between the fourth level and degenerate second and third levels with occupation inversion 6.5 %, the transition frequency being $\Omega = 14.3$ eV. Assuming the electron beam brightness $B = 1.7 \cdot 10^{19}$ A m^{-2} corresponding to [2] and beam focused within Lindhard angle one get from (4) for the beam susceptibility $\chi_b = 4.6 \cdot 10^{-13}$. The largest instability increment can be observed when roots of (8) left hand side are closest to each other, that takes place at the edge of the Darwin table, see Fig 1. For the considered case from (8) one can estimate instability increment as

$$\mathrm{Im}k_z^{(r)} = \frac{\omega}{c}\frac{\chi_b}{2\mathrm{Im}\chi_0(1-e^{-W})} \tag{10}$$

here we have taken use of the fact that for even reflexions $\mathrm{Im}\chi_H = e^{-W}\mathrm{Im}\chi_0$ where W is Debye-Waller factor. One can see that accounting for Bragg diffraction leads to increase of instability increment due to increase of effective absorption length, an effect being similar to anomalous transmission Borrmann effect. Applying the boundary conditions and assuming the crystal slab thickness 200 µm one can see in a narrow angle range an essential increase of radiation intensity compared to spontaneous radiation case for the same parameters. To describe this process beyond the exponential growth regime and more realistically one has to take the dechanneling effect into account and analyze the complete system (3), that will be the subject of further investigations.

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