

# THREE-DIMENSIONAL ANALYSIS OF THE SURFACE MODE SUPPORTED BY A REFLECTION GRATING \*

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## Abstract

In a Smith-Purcell Free-Electron Laser (SP-FEL), the electron beam interacts with the surface mode supported by a metallic reflection grating to produce coherent radiation. All the previous analyses of SP-FEL had considered the localization of the surface mode only in the direction perpendicular to the grating surface and assumed translational invariance along the direction of grooves of the grating. In this paper, we include the localization of the surface mode along the direction of grooves as well and study the three-dimensional structure of the surface mode in order to include diffraction effects in the analysis of SP-FELs. Full three-dimensional Maxwell-Lorentz equations are derived for the self-consistent nonlinear analysis of SP-FELs.

## INTRODUCTION

Smith-Purcell Free-Electron Laser (SP-FEL) is seen as an attractive option for a compact coherent terahertz source using low energy electron beam. In an SP-FEL, coherent electromagnetic radiation is generated due to the interaction of an electron beam with the surface electromagnetic mode supported by a reflection grating. Several authors have recently studied this interaction using analytical as well as numerical techniques [1-4]. In all the previous analyses, the three-dimensional effects have been either ignored or included only approximately. This is because these analyses consider the interaction of the electron beam with the two-dimensional surface mode, where the electromagnetic field has no variation along the direction of grooves of the reflection grating. The two-dimensional surface mode is therefore not localized in the direction of grooves, although it is localized in the direction perpendicular to the grating surface. We call such surface modes as nonlocalized surface modes in this paper. The diffraction of surface mode along the direction of grooves, which affects the overlap with the electron beam and hence the build-up of power is therefore not included in these analyses. It is important to include three-dimensional effects in the analysis to accurately study the performance of the system and also to accurately calculate the start current, which is the threshold electron beam current for coherent growth of power. In this paper, we study the three-dimensional surface mode, which is localized in both the transverse directions that are perpendicular to the direction of propagation. We also discuss the coupled Maxwell-Lorentz equation to describe the

interaction of the electron beam with the three-dimensional surface mode.

In the next section, we discuss the dispersion relation of an off-axis nonlocalized surface mode supported by a reflection grating. The construction of three-dimensional localized surface mode using a combination of off-axis nonlocalized modes is discussed in the following section. Maxwell-Lorentz equation for the interaction of the electron beam with the three-dimensional surface mode is discussed after that and finally, we present some conclusions in the last section.

## DISPERSION RELATION OF A SURFACE MODE PROPAGATING OFF-AXIS

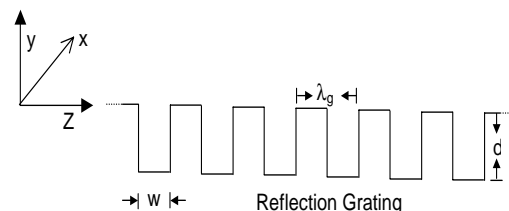


Figure 1: Schematic of a rectangular reflection grating. The top surface of the grating is in the plane  $y = 0$ .

Figure 1 shows the schematic of a rectangular metallic reflection grating having period  $\lambda_g$ , groove depth  $d$ , and groove width  $w$ . We want to study the self-consistent electromagnetic field supported by this structure. All the previous analyses of this problem assumed the system to have translational invariance in the  $x$ -direction and hence these are two-dimensional analyses. Here, we assume an  $\exp(ik_x x)$  type variation in EM field along the  $x$ -direction. In order to find out the dispersion relation of the surface mode, we follow our earlier approach [3, 5], where the surface mode appears in terms of singularities of the reflection matrix  $\mathcal{R}$ . The EM field in the region  $y > 0$  is composed of the incident and reflected wave having the following Floquet-Bloch expansion for the  $H$ -polarization:

$$H_x^I = \sum_{n=-\infty}^{+\infty} A_n^I \exp(ik_n z + ik_x x - ip_n y - i\omega t), \quad (1)$$

$$H_x^R = \sum_{n=-\infty}^{+\infty} A_n^R \exp(ik_n z + ik_x x + ip_n y - i\omega t). \quad (2)$$

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Here  $n$  is the spectral order,  $A_n^R = \sum \mathcal{R}_{nm} A_m^I$ ,  $k_n = k_z - nk_g$ ,  $k_z = k/\beta$ ,  $k = \omega/c$ ,  $k_g = 2\pi/\lambda_g$ ,  $p_n = i\Gamma_n = \sqrt{k^2 - k_x^2 - k_n^2}$ , and the sign of the square root is chosen such that  $[\text{Re}(p_n) + \text{Im}(p_n)] \geq 0$ , which is essentially the outgoing wave condition [6]. The phase velocity of the zeroth-order component along the  $z$ -axis is  $\beta$  in the unit of the speed of light  $c$ . Note that the plane wave components described by Eqs. (1-2) are in general, propagating off-axis in the  $xz$  plane. The total electromagnetic field  $\vec{E}$  and  $\vec{H}$  in the region  $y > 0$  is obtained by combining the contribution from the incident and reflected waves. In addition to  $H_x$ , the EM field will have  $E_z$ ,  $E_y$ ,  $H_z$  and  $H_y$  components also. Defining  $\vec{E} = \vec{\mathcal{E}}(y, z) \exp(ik_x x - i\omega t)$  and  $\vec{H} = \vec{\mathcal{H}}(y, z) \exp(ik_x x - i\omega t)$ , these components are given by [7]

$$(k^2 - k_x^2)\mathcal{E}_z = -i\omega\mu_0(\partial\mathcal{H}_x/\partial y), \quad (3)$$

$$(k^2 - k_x^2)\mathcal{E}_y = i\omega\mu_0(\partial\mathcal{H}_x/\partial z), \quad (4)$$

$$(k^2 - k_x^2)\mathcal{H}_z = ik_x(\partial\mathcal{H}_x/\partial z), \quad (5)$$

$$(k^2 - k_x^2)\mathcal{H}_y = ik_x(\partial\mathcal{H}_x/\partial y), \quad (6)$$

where  $\mu_0$  is the permeability of vacuum. Note that since we are considering  $H$ -polarization as opposed to  $E$ -polarization due to its strong interaction with co-propagating electron beam, we take  $E_x = 0$ .

The electromagnetic field inside the grooves can be expressed as a superposition of cavity modes, and the expression for  $\mathcal{H}_x$  in the  $M^{\text{th}}$  groove ( $M\lambda_g + b < z < M\lambda_g + \lambda_g$ ), where  $b = \lambda_g - w$  can be written as [8]

$$\mathcal{H}_x^{(M)} = \sum_{s=0}^{\infty} A_s^{(M)} \cos[q_s(z - z_M)] \cos[Q_s(y + d)], \quad (7)$$

where  $q_s = \pi s/w$ ,  $Q_s = [k^2 - k_x^2 - q_s^2]^{1/2}$ ,  $z_M = M\lambda_g + b$ . The remaining components of EM field inside the groove can be determined in the same way as described above by Eqs. (3-6). In the metallic portion of the grating, the electromagnetic field can be assumed to be vanishing. The following expression for the reflection matrix  $\underline{\mathcal{R}}$  is obtained by satisfying the boundary condition at the interface  $y=0$  for  $E_z$  and  $H_x$ :

$$\underline{\mathcal{R}} = (\underline{I} + \underline{Z})^{-1}(\underline{I} - \underline{Z}), \quad (8)$$

where  $\underline{I}$  is the identity matrix and  $\underline{Z}$  is the impedance matrix given by

$$Z_{mn} = -\frac{w}{\lambda_g} \frac{1}{\Gamma_m} \sum_{s=0}^{\infty} \frac{Q_s \tan(Q_s d)}{g_s} \times \mathcal{L}(p_n; s) \mathcal{L}^*(p_m; s). \quad (9)$$

Here,  $\mathcal{L}^*$  is the complex conjugate of  $\mathcal{L}$ ,  $g_0 = 1$ ,  $g_{s \neq 0} = 1/2$ , and  $\mathcal{L}$  is given by

$$\mathcal{L}(p_m; s) = e^{ik_m b} \frac{1}{2} \left[ e^{-i\theta_-} \frac{\sin \theta_-}{\theta_-} + e^{-i\theta_+} \frac{\sin \theta_+}{\theta_+} \right],$$

where  $\theta_{\pm} = (-wk_m \pm \pi s)/2$ . The above expression for  $\underline{\mathcal{R}}$  has the same form as given in Ref. [8] except that it is now generalized to include non-zero value of  $k_x$ . We make an important observation here that the effect of introducing a finite value of  $k_x$  is that  $\omega$  in earlier expression simply gets replaced with  $\sqrt{\omega^2 - c^2 k_x^2}$ . With the help of this replacement rule, we can use the earlier calculation performed for the  $k_x = 0$  case even for a finite  $k_x$  case.

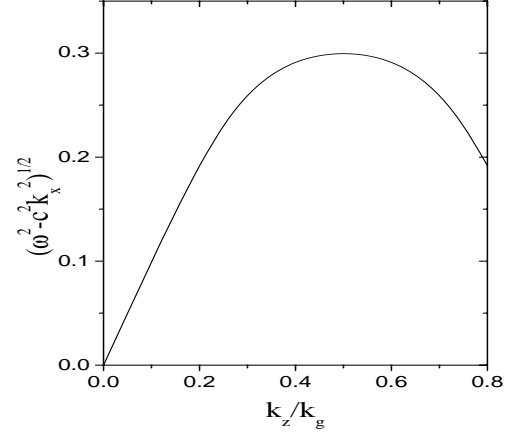


Figure 2: Typical dispersion relation for a rectangular reflection grating for a surface mode propagating off-axis.

Next, we discuss the dispersion relation of the surface mode. The surface mode appears as a singularity in the reflection matrix. For example, for a given value of  $\omega$  and  $k_x$ , we can find a value of  $k_z$  for which the reflection matrix becomes singular. This means that reflected components given by Eq. (2) are supported self-consistently by the grating without the need of incident waves. Also, the reflected components corresponding to different values of  $n$  in Eq. (2) add in a certain fixed ratio of amplitudes such that the boundary conditions are satisfied on the grating surface [3]. In this way, by studying the singularity of  $\underline{\mathcal{R}}$ , we can find out the dispersion relation of the surface mode. We have earlier discussed the calculation of dispersion relation for  $k_x = 0$  case in Refs. [3,5]. The same calculation can be used to get the dispersion relation for a finite  $k_x$  case, using the replacement rule that we have discussed in this section. Fig. 2 shows a typical dispersion relation plotted for a certain set of grating parameters. For a given value of  $\omega$  and  $k_x$ , there is a certain fixed value of  $k_z$  and also the values of  $A_n/A_0$  for all values of  $n$  are fixed and can be calculated. As has been discussed earlier [1, 3], the group velocity of the surface mode co-propagating with low energy electron beam is negative, meaning that the energy flows backward if the phase velocity is in the forward direction.

Hence, in this section, we have discussed surface mode which propagates off-axis, but is still nonlocalized in the  $x$  direction. In the next section, we use this to construct a set of fully localized surface modes.

### THREE-DIMENSIONAL STRUCTURE OF THE LOCALIZED SURFACE MODE

In the last section, we have discussed the surface mode that is composed of plane waves which propagate, in general, off-axis in the  $xz$  plane. We can combine such surface modes with suitable weight function in  $k_x$  to obtain a mode that is localized in the  $x$  direction as follows

$$E_z^T = \sum_n \int dk_x A_n(k_x) \exp(ik_n z + ik_x x - \Gamma_n y). \quad (10)$$

Note that it is here understood that all the field quantities have  $\exp(-i\omega t)$  type time dependence. Here,  $E_z^T$  stands for the total longitudinal electric field and  $\Gamma_n$  is real, meaning that the field decays and is localized in the  $y$  direction. Note that for a given  $k_x$ , the relative magnitudes of the amplitude  $A_n$  (i.e., the ratio  $A_n/A_0$  for all values of  $n$ ) as well as the relation between  $k_z$  and  $\omega$  can be calculated as mentioned in the last section. The  $k_z$  and  $\Gamma_n$  are therefore functions of  $k_x$  in the above integral for a given value of  $\omega$ . In the above expression, only the zeroth-order component corresponding to  $n = 0$  term interacts strongly with the co-propagating electron beam and we will therefore focus on this term only in the remaining of the paper. However, all other components are present there with an amplitude in a fixed ratio with the amplitude of the zeroth-order component such that boundary conditions are satisfied at the grating surface.

Let us introduce the angle  $\phi$  in the  $xz$  plane via  $k_x = k_z \sin \phi$ . Under the paraxial approximation  $\phi \ll 1$ , we obtain the following expressions for the  $\phi$ -dependence of  $k_z$  and  $\Gamma_0$ :

$$k_z(\phi) = k_z \left(1 + \frac{\phi^2}{2\beta\beta_g}\right), \quad (11)$$

$$\Gamma_0(\phi) = \Gamma_0 + \frac{k_z^2 \phi^2}{2\Gamma_0} \left(1 + \frac{1}{\beta\beta_g}\right), \quad (12)$$

where we have simplified the notations by writing  $k_z = k_z(0)$  and  $\Gamma_0 = \Gamma_0(0)$ . Here  $\beta_g$  is the magnitude of the group velocity ( $d\omega/dk_z$  for  $k_x = 0$ ) of the surface mode in the unit of  $c$ . As mentioned earlier, the group velocity is negative. We can substitute the above expressions for  $k_z$  and  $\Gamma_0$  in the Eq. (10) and only retain the  $n = 0$  term and get the following expression for the field in the zeroth-order component:

$$E_z^0 = e^{-\Gamma_0 y} e^{ik_z z} \int \underbrace{A_0(\phi) e^{i \frac{k_z \phi^2 z}{2\beta\beta_g}} e^{-\frac{k_z^2 \phi^2}{2\Gamma_0} \left(1 + \frac{1}{\beta\beta_g}\right) y}}_{\times e^{ik_x \phi x} d\phi}. \quad (13)$$

We note that  $E_z^0$  appears as a Fourier transform in  $\phi$  of the underbraced term in the above expression. We can take the orthonormal set of Gauss-Hermite functions for  $A_0(\phi)$  and obtain a set of Gauss-Hermite orthonormal surface modes which are localized in the  $x$  direction. This is exactly the same way in which one can get the localized FEL Theory

Gauss-Hermite modes for a laser beam in free space [9]. Here, we consider only the fundamental Gaussian mode by choosing  $A_0(\phi) = \exp(-\phi^2/4\sigma_\phi^2)$  for which we obtain the following expression for the rms beam size  $\Sigma_x$  [10]

$$\Sigma_x^2(y; z) = \Sigma_x^2(y; 0) + \Sigma_\phi^2(y) z^2. \quad (14)$$

Note that the above equation is in the form of paraxial diffraction with a waist at  $z = 0$ , the rms waist beam size of  $\Sigma_x(y; 0)$ , and an rms diffraction angular divergence of  $\Sigma_\phi(y)$ . The quantities on the right-hand side of Eq. (14) are determined by the following relations:

$$\Sigma_x^2(y; 0) = \sigma_x^2 + \frac{y}{2\Gamma_0} \left(1 + \frac{1}{\beta\beta_g}\right), \quad (15)$$

$$\sigma_x \sigma_\phi = \frac{1}{2k_z}, \quad (16)$$

$$\Sigma_x(y; 0) \Sigma_\phi(y) = \frac{1}{2k_z \beta |\beta_g|} = \frac{\lambda}{4\pi |\beta_g|}. \quad (17)$$

These reduce to the well-known relations between the rms size and angular divergence in free space when  $|\beta_g| = 1$ . Eq. (14) can also be written in a form familiar in paraxial optics discussions:

$$\Sigma_x^2(y; z) = \frac{\lambda}{4\pi |\beta_g|} \left(Z_R + \frac{z^2}{Z_R}\right), \quad (18)$$

where the Rayleigh range  $Z_R$  is given by

$$Z_R = \frac{4\pi |\beta_g|}{\lambda} \Sigma_x^2(y; 0). \quad (19)$$

We have thus derived in this section the three-dimensional structure of fully localized surface mode. The fundamental Gaussian mode is discussed in detail and the analysis can be easily extended to derive the structure of higher order Gauss-Hermite surface modes. Note that compared to Gauss-Hermite modes propagating in free space, the wavelength  $\lambda$  is here replaced with  $\lambda/\beta_g$ .

### THREE-DIMENSIONAL MAXWEL-LORENTZ EQUATIONS

We now discuss the interaction of the localized mode that we discussed in the last section with the co-propagating electron beam. For the two-dimensional case, where the system is assumed to have translational invariance in the  $x$  direction, we had earlier derived the coupled nonlinear Maxwell-Lorentz equation for the interaction of the surface mode with the sheet electron beam [3]. Using the Maxwell equation with the source term and using the slowly varying envelope approximation and the paraxial approximation, we can write down the equation for the evolution of the electromagnetic field given by Eq. (13). Leaving the details of the derivation to another publication [11], we present here the final result:

$$\begin{aligned} \frac{\partial E_z}{\partial z} - \frac{1}{2i\beta\beta_g k_z} \frac{\partial^2 E_z}{\partial x^2} - \frac{1}{\beta_g c} \frac{\partial E_z}{\partial t} \\ = \frac{Z_0 \chi}{2\beta\gamma} \int dy j_z e^{-\Gamma_0 y} \langle e^{-i\theta} \rangle, \end{aligned} \quad (20)$$

where  $Z_0 = 377\Omega$  is the characteristic impedance of free space,  $\chi$  is the residue of the singularity associated with the surface mode as defined in Ref. [3],  $j_z$  is the electron volume current density at the given location,  $\theta$  is the phase of the electron and  $\langle \cdot \cdot \cdot \rangle$  denotes averaging over electrons. Note that  $E_z$  is the amplitude of the electric field in the zeroth-order component of the surface mode at the grating surface, i.e.,  $y = 0$ . Once  $E_z$  is known, one can calculate  $A_0(\phi)$  using Eq. (13) and then as discussed earlier in this paper, we can calculate  $A_n(\phi)$  for all  $n$ . Substituting these in Eq. (10), we get the total electromagnetic field. Note that by construction, this electromagnetic field satisfies the boundary condition on the grating surface and also evolves due to interaction with co-propagating electron beam as given by Eq. (20). It is interesting to observe that the structure of this equation is similar to that for the case of conventional FELs. The second term on the left side this equation represents diffraction and compared to the conventional FEL case, here  $\lambda$  is replaced with  $\beta_g \lambda$ . This is same as we observed in the last section, where the same replacement occurs in the formula for the Rayleigh range in Eq. (19).

The equation for the evolution of phase and energy of the electrons, as derived earlier [3] are given by

$$\frac{1}{\beta c} \frac{\partial \gamma_i}{\partial t} + \frac{\partial \gamma_i}{\partial z} = \frac{e E_z}{m c^2} e^{i\psi_i} + c.c., \quad (21)$$

$$\frac{1}{\beta c} \frac{\partial \theta_i}{\partial t} + \frac{\partial \theta_i}{\partial z} = \frac{k}{\beta^3 \gamma^2} \frac{(\gamma_i - \gamma_p)}{\gamma_p}, \quad (22)$$

where  $\gamma_p$  is the energy of the electron resonant with the surface mode in the unit of rest mass energy,  $\gamma_i$  is the energy of the  $i^{\text{th}}$  electron in the unit of rest mass energy and  $\theta_i$  is the phase of  $i^{\text{th}}$  electron. Note that here we have ignored space-charge term in Eq. (21) for simplicity. Eqs. (20-22) are the coupled three-dimensional time-dependent Maxwell-Lorentz equations, which describe the interaction between the surface mode and the electron beam. If there are focusing forces, there will be equations for the evolution of transverse dynamical variables of electrons, in addition to Eqs. (21-22).

Finally, we give the expression for the power flowing in the surface mode in the backward direction. In general, power will flow along  $x$  direction also in addition to  $z$  direction in 3-D case. However, under paraxial approximation, we can assume that power flowing along the  $x$  direction is not very significant. The expression for the power  $P$  flowing along the (negative)  $z$  direction, which is further generalization of the expression obtained for 2-D case in Refs. [3,12] is given by

$$P = 2 \frac{\beta \gamma}{Z_0 \chi} \int |E_z|^2 dx. \quad (23)$$

Note that the above expression is for the total power corresponding to EM field in all the components corresponding to different values of  $n$  in Eq. (10).

FEL Theory

## CONCLUSIONS

In this paper, we have discussed the three-dimensional surface electromagnetic modes supported by a reflection grating that are localized along the direction of grooves as well as in the direction perpendicular to the grating surface. We have then discussed the nonlinear three-dimensional time-dependent coupled Maxwell-Lorentz equations for the interaction of the surface mode with the electron beam. These equations can be numerically solved to study the evolution of power in an SP-FEL taking diffraction effects into account, which has so far not been accurately studied. We can linearize the corresponding Maxwell-Vlasov equation and solve it approximately to get an analytic expression for start current taking three-dimensional effects into account. This will be taken up in the future.

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