Compact Short-Wavelength Free-Electron Laser

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A new nonclassical model is proposed for the radiation from electrons skimming over and colliding at grazing incidence with a conducting diffraction grating. Radiation originating from induced surface currents and bremsstrahlung is amplified as it passes through spatially modulated wave functions above the grating. The predicted magnitude and dependence on electron beam thickness agree with experiments at visible wavelengths and suggest the possibility of a compact x-ray laser.

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The radiation from electrons interacting with a conducting diffraction grating has been discussed several times in the past forty years. Smith and Purcell[1] originally attempted to explain the light generated by an electron passing over the grating as being due to the oscillating dipoles formed by the electron and its image charge. Salisbury[2] proposed that the much enhanced radiation he observed when the electrons impacted the grating was due to accelerations of the electrons as they passed through periodic space-charge sheets above the grating formed from reflected electrons. Elaborations of the Smith-Purcell explanation have been provided by several investigators, including de Francia,[3] who explained the radiation in terms of the transformation of evanescent waves from the electron into propagating waves at the grating, Barnes and Dedrick,[4] who performed a Green's-function calculation, and McDaniel *et al.*,[5] who derived the radiation characteristics in terms of induced surface currents. Salisbury's space-charge-sheet mechanism has been analyzed by Gover and Yariv[6] and by McDaniel, Chang, and Salisbury,[7] who found that the accelerations of the electrons in the space-charge sheets are too small to contribute appreciable radiation. Recently, an alternative explanation of the radiation was proposed by Chang and McDaniel[8] in terms of bremsstrahlung from a periodic structure.

None of the foregoing explanations appear adequate to explain the recent experimental results of Shih *et al.*[9] In these experiments, the radiation was found to be 10000 times more intense than that predicted by the Smith-Purcell–Salisbury related explanations, and 100 times more intense than that predicted by the bremsstrahlung explanation. Moreover, the angular distribution did not appear to be that predicted by the Smith-Purcell–Salisbury explanations, although it did peak at the angle predicted by the bremsstrahlung calculation. The most striking feature of the experiments of Shih *et al.*, however, was the finding that the intensity increased with thickness of the electron beam to thicknesses 1000 times the grating spacing, and then saturated as the thickness was further increased. The appreciable contribution of electrons at great distances from the grating confirmed earlier results of Salisbury,[2,10] and was what led him originally to propose the space-charge-sheet explanation for the radiation enhancement.

The purpose of this Letter is to propose a new quantum-mechanical explanation for the radiation from electrons impacting a conducting diffraction grating at skimming incidence, and to point out that the proposed mechanism should make possible the operation of compact x-ray lasers. In the proposed mechanism, amplification of the bremsstrahlung from electrons impacting the grating and the conventional Smith-Purcell radiation occurs in the region above the grating. This amplification results from the interaction of the radiation with the portion of an electron's wave function above the grating with the portion of an electron's wave function above the grating which results from diffraction off of the microcrystals comprising the grating. This diffracted wave function is spatially modulated with a period parallel to the grating equal to the grating period. This modulation makes possible the conservation of momentum and energy in the process of absorbing or emitting a photon.

To see the amplification mechanism, consider an electron of mass m, charge e, wave number k_0, and energy $E_0=\hbar^2k_0^2/2m$ incident at skimming incidence on a grating of period $2\pi/k_g$ made of a conducting cubic lattice of lattice constant a.

Take the grating to occupy the space $y<0$ with its grooves oriented along the z direction, and take the incident electron to be described by

$$\Psi_I=Be^{ik_0x}e^{-iE_0t/\hbar}, \quad -d<y<y_{\max}, \tag{1}$$

where B is a normalization constant and $2\pi\hbar$ is Planck's constant. Here, the depth of penetration into the grating surface, and the maximum extent of the electron's wave formation above the grating surface $y_{\max}$, depend on the electron optics defining the beam of electrons incident on the grating at a skimming angle. In the Born approximation, if the electron impacts the grating at the x coordinate x_g, and at $z=0$, then at a point (x,y,z) far above the grating surface the scattered wave function $\Psi_s(\mathbf{r},t)$ is

$$\Psi_s=\frac{2mZe^2B}{\hbar^2(\Delta k)^2r}e^{ik_0r}e^{ik_0x_g}\sum_j e^{-i\Delta\mathbf{k}\cdot(\mathbf{r}_j-x_g\mathbf{i}_x)}, \tag{2}$$

where

$$r^2=(x-x_g)^2+y^2+z^2 \tag{3}$$

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and $\Delta k = |\Delta \mathbf{k}|$, with

$$\Delta \mathbf{k} = k_0 \left\{ \left(\frac{x - x_g}{r} - 1 \right) \iota_x + \frac{y}{r} \iota_y + \frac{z}{r} \iota_z \right\} \quad (4)$$

and $\mathbf{r}_j$ designates the location of the accessible Coulomb scatterers of charge z.

For the cubic lattice oriented along the x,y,z axes, strong resonances occur at the Bragg angles:

$$\Delta k_i a = 2\pi n_i, \quad i = x,y,z , \quad (5)$$

with the width of the resonances inversely proportional to the number of scatterers along the x,y,z axes, $N_x + 1$, $N_y + 1$, and $N_z + 1$,

$$\delta(\Delta k_i) = 2\pi / a(N_i + 1), \quad i = x,y,z . \quad (6)$$

Because of the strong enhancement of Ψ_s at the Bragg angles, and because of the $(\Delta k)^{-2}$ factor in the expression for Ψ_s, we shall make the approximation that Ψ_s is due only to scattering into the first Bragg peak $\Delta k_y a = 2\pi$, $\Delta k_x = \Delta k_z = 0$. In that case, $y = (x - x_g)\Theta_D$, and we may write

$$\Psi_0(x,y,z=0,t) = \Psi_I + \Psi_s = B e^{ik_0 x}\{1 + (\xi_1/y) e^{ik_B \Theta_D y}[1 + \xi_2 \cos k_g (x - y/\Theta_D)]\} e^{-iE_0 t/\hbar} , \quad (7)$$

where

$$\xi_1 = \frac{2mZe^2 \Theta_D (N_x + 1)(N_y + 1)(N_z + 1)}{\hbar^2 (2\pi/a)^2} , \quad (8)$$

$$\xi_2 = \frac{\sin(aN_x k_g/2)(-1)^{N_x n_x}}{\sin(a k_g/2)(N_x + 1)} \to \left(\frac{N_x}{N_x + 1} \right) (-1)^{N_x n_x} \text{ when } \frac{N_x k_g a}{2} \ll 1 , \quad (9)$$

and

$$\Theta_D = 2\pi / k_0 a = \lambda_0 / a \ll 1 . \quad (10)$$

For an electron beam with considerable width in the z direction, the factors N_x, N_y, and N_z in Ψ_s can be quite large. But there is a limitation on their magnitudes due either to the requirement that the angle subtended at x, y, and z by the scattering volume be less than the resonance widths, or by the requirement that $N_x a$ and $N_y a$ be less than the range of the electrons in the material lattice comprising the grating. In the former case, the geometry requires

$$(N_y + 1)^2 a^2 = (N_z + 1)^2 a^2 \le r\lambda_0 = y\lambda_0/\Theta_D = ya \quad (11)$$

and

$$(N_x + 1)(N_y + 1) a \le ar = ay/\Theta_D = a^2 y/\lambda_0 , \quad (12)$$

where $\lambda_0 = 2\pi/k_0$. On the other hand, if the $(N_x + 1)a$ and $(N_y + 1)a$ limitations imposed by the resonance-width requirement are larger than the range of the electron in the grating material $R(k_0)$, then the correct limit is approximately

$$(N_x + 1)a = (N_y + 1)a \le R(k_0) , \quad (13)$$

$$(N_z + 1)^2 a^2 \le r\lambda_0 = y\lambda_0/\Theta_D = ya . \quad (14)$$

Consider now a radiation field propagating through an ensemble of electrons having wave functions of the form of Eq. (7) for diffraction off a grating comprising a single crystal. Specifically, we take a field of the form

$$\mathbf{A} = \mathbf{A}_1 \cos(\omega t - Kx\cos\Theta - Ky\sin\Theta) , \quad (15)$$

with

$$\mathbf{A}_1 = -A_1 \sin\Theta \iota_x + A_1 \cos\Theta \iota_y \quad (16)$$

and $\omega = Kc$. The perturbation Hamiltonian is

$$H' = (ie\hbar/mc)\mathbf{A}\cdot\nabla \quad (17)$$

and the probability per unit time of making a transition from the state Ψ_0 of Eq. (7) to a final state Ψ_F of the same form is

$$\Gamma_{0F} = (2\pi/\hbar)|M_{0F}|^2 \delta(E_F - E_0 \pm \hbar\omega) , \quad (18)$$

where

$$M_{0F} = \int d^3x\, \Psi_F^* H' \Psi_0 . \quad (19)$$

For wave functions of the form of Eq. (7), only the portion containing the factor $\xi_1[1 + \xi_2 \cos k_g (x - y/\Theta_D)]$ contributes to nonzero M_{0F}. The energy-conservation requirement gives, with $v_0 = \hbar k_0/m$,

$$\omega = k_g v_0 [1 - (v_0/c)\cos\Theta]^{-1} , \quad (20)$$

$$\Delta k = \pm \omega/v_0 = \pm k_g [1 - (v_0/c)\cos\Theta]^{-1} . \quad (21)$$

The nonzero matrix element M_{0F} is

$$M_{0F} = -\frac{e v_0 A_1}{c y^2} \xi_1^2 \xi_2 [-\sin\Theta + \Theta_D \cos\Theta] . \quad (22)$$

The rate at which the energy ϵ in the wave is growing in space is given by $\kappa = d(\ln\epsilon)/ds$:

$$\kappa = [f(k_0) - f(k_0 - \Delta k)] \frac{32\pi^3 k_0^3 e^2}{mc\omega y^4} \xi_1^4 \xi_2^2 [-\sin\Theta + \Theta_D \cos\Theta]^2 , \quad (23)$$

where $f(k_0)dk_0$ denotes the number of incident electrons per unit volume with wave numbers in the range $dk_B \iota_x$ at $k_B \iota_x$.

For electrons thermionically emitted from a cathode of work function E_w, and subsequently accelerated through a potential Φ to an energy $E_\Phi = e\Phi$, if the beam density is low enough for no randomizing collisions to occur outside the cathode and for no Child's-law limitation of current, we may write $f(k_0) = (\hbar/m)^3 F(v_0)$ where

$$F(v_0) = \begin{cases} n_0 \left(\dfrac{\alpha}{\pi}\right)^{3/2} \dfrac{v_0 \exp\{-\alpha[v_0^2 - (2/m)(E_\Phi - E_w)]\}}{[v_0^2 - (2/m)(E_\Phi - E_w)]^{1/2}}, & v_0 > \left(\dfrac{2E_\Phi}{m}\right)^{1/2}, \\ 0, \quad v_0 < \left(\dfrac{2E_\Phi}{m}\right)^{1/2}. \end{cases} \tag{24}$$

In this expression n_0 is the density of electrons in the cathode, and $\alpha = m/2k_B T_c$ with k_B denoting Boltzmann's constant and T_c the cathode temperature. The density of electrons over the grating is approximately

$$n_g = (n_0/2\sqrt{\pi})(E_w/k_B T_c)^{1/2} e^{-2\alpha E_w/m}, \tag{25}$$

and in terms of n_g

$$\kappa = \frac{32\pi^2 n_g v_0^4 e^2 \alpha}{c\omega E_w y^4} \xi_1^4 \xi_2^2 [-\sin\Theta + \Theta_D \cos\Theta]^2, \tag{26}$$

when v_0 is taken to be $(2E_\Phi/m)^{1/2}$.

If the grating is not made from a single crystal, but instead is made of material comprising small microcrystallites of random orientation, the diffracted wave function resembles that of a powder. The primary peak still occurs near the first Bragg peak Θ_D, but the width instead of being of the order of $\Theta_D/(N_i+1)$ is of the order of Θ_D due to the random orientations of the microcrystallites. The number of microcrystallites contributing to the Ψ_s at any point is limited by the requirement that the path in the grating of an incident electron and a diffracted electron cannot exceed the range $R(k_0)$ of the electron in the material. The result of these two effects if that for a grating comprising microcrystallites,

$$\kappa(\text{microcrystallites}) = \frac{[R(k_0)]^6 \Theta_D^2}{a^6 (N+1)^{10}} \kappa(\text{single crystal}) \tag{27}$$

where $(N+1)^3$ is the number of scattering centers in a microcrystallite. The spatial growth rate of radiation above a grating etched into a microcrystalline substrate is much less than that for a grating etched into a single crystal, if $(N+1)a$ is anywhere near as large as the range of the electron in the grating.

For scattering from a single crystal, the y at which the range limitation takes over from the resonance width limitation, y_c, is obtained by equating the two. This gives

$$y_c = [R(k_0)]^4 \lambda_0^2 / a^5. \tag{28}$$

For $y < y_c$, $\xi_1 \sim y^{3/2}$ so that $\kappa \sim y^2$. For $y > y_c$, $\xi_1 \sim y^{1/2}$ so that $\kappa \sim y^{-2}$. Accordingly, the intensity is

$$I \sim \exp(c_1 y^3), \quad y < y_c, \tag{29}$$

$$I \sim \exp(-c_z/y), \quad y > y_c, \tag{30}$$

where c_1 and c_2 are constants. For the microcrystallite case,

$$I \sim \exp(-c_3/y^3), \tag{31}$$

where c_3 is a constant.

Both Eqs. (30) for the amplification above a grating formed from a single crystal and Eq. (31) for the amplification above a grating formed from randomly oriented microcrystals show saturation at large y. The saturation sets in much more abruptly in the microcrystalline case. The large contribution of electrons at distances from the grating surface several thousand times the grating period has long been puzzling. In contrast to the exponential dropoff of Smith-Purcell radiation with electron distance, the contribution of Eq. (23) drops off as a power law due to the slow decrease of the diffracted wave function with distance from the surface.

In the recent experiments of Shih *et al.*, the radiation intensity was found to increase with electron beam thickness to several thousand times the grating period, and then to saturate on further increase in thickness. This appears to be consistent with the behavior predicted by Eq. (31).

It is interesting that the amplification obtained here is not what one would predict in a classical calculation of amplification in a slow-wave structure comprising periodically spaced space-charge sheets. At the low electron densities in the experiments of Salisbury and Shih *et al.* (10^4–10^6 cm^{-3}), the plasma frequency is less than 10^{-9} of the frequency of the visible radiation produced. The resulting effect on wave propagation through the structure is quite negligible. In the corresponding absence of appreciable spatial sidebands in the propagating radiation waves, formation of $\mathbf{j}\cdot\mathbf{E}$, where $\mathbf{j}$ is the current density produced by the radiation electric field $\mathbf{E}$, shows no secular exchange of energy between the beam electrons and the field.

For reasonable parameters, the predicted magnitude of the amplification and the behavior with increasing beam thickness of the radiation intensity appear to be consistent with the recent experiments of Shih *et al.* at visible wavelengths. In these experiments, a wide 10^6-cm^{-3} beam of 100-keV electrons impacted at skimming incidence a 2.5-cm platinum diffraction grating with a period of 0.5 μm. The intensity of radiation produced was found to increase with beam thickness to a thickness of about 0.5 mm before saturation. The measured intensity was found to be 10^4 more intense than Smith-Purcell radiation and 10^2 more intense than that predicted by a periodic bremsstrahlung model. The bremsstrahlung model did, however, predict the observed peak in radiation intensity at $\Theta = 75°$. An increase in intensity by another factor of 10^2 would be consistent with Eq. (31) for y increasing from 80 μm to 0.4 mm, if the typical size of the microcrystallites is of the order of 300 Å on a side. Since the large-y approximation was used in deriving Eq. (31), and since 80 μm is 16 times the expected range of a 100-keV electron in platinum, it is reasonable to expect Eq. (31) to apply for y larger than this value.

The expressions of this paper have been derived ignoring nonlinear terms, so care must be exercised in applying them to cases where the parameters correspond to very large ξ_1 (for the Shih *et al.* experiments, $\xi_1 \sim 10^{-2}$). In addition, the expressions have been derived for the nonrelativistic case. Nevertheless, because of the properties of Coulomb scattering, relativistic expressions for κ are not too different from our expressions if relativistic masses are used wherever the electron rest mass m appears. With Θ_D inversely proportional to the relativistic momentum, and with the range of electrons in materials increasing as a low power of energy, the spatial growth rate κ for the single-crystal case is essentially independent of electron energy except for the $\omega^{-1} \times [-\sin\Theta + \Theta_D \cos\Theta]^2$ dependence. This suggests that the mechanism should be operable in the x-ray range of wavelengths, using relativistic electrons. Nonrelativistic electrons could also be used with gratings of smaller period than the 5000 Å used in the visible wavelength experiments: The resulting wavelengths would be comparable to the shorter grating periods. However, use of relativistic electrons makes it possible to obtain much smaller wavelengths with larger grating periods. Thus, for relativistic electrons, Eq. (20) for ω becomes, when $\Theta = 0$,

$$\omega \rightarrow k_g v_0/(1 - v_0/c) \approx k_g c (E_0/mc^2)^2 . \quad (32)$$

In that case, 5-MeV electrons impacting at grazing incidence a grating with 100-Å period should provide 1-Å x rays which can be substantially amplified by the diffracted electrons above the grating. Equation (26) shows that operation at $\Theta = 0$ reduces the spatial growth rate κ by Θ_D^2. This is partially compensated by the longer available path length along the grating for amplification, and would certainly be more than compensated by using a grating etched from a single crystal instead of randomly oriented microcrystallites.

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