Analytic theory of soft x-ray diffraction by lamellar multilayer gratings

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Abstract: An analytic theory describing soft x-ray diffraction by Lamellar Multilayer Gratings (LMG) has been developed. The theory is derived from a coupled waves approach for LMGs operating in the single-order regime, where an incident plane wave can only excite a single diffraction order. The results from calculations based on these very simple analytic expressions are demonstrated to be in excellent agreement with those obtained using the rigorous coupled-waves approach. The conditions for maximum reflectivity and diffraction efficiency are deduced and discussed. A brief investigation into p-polarized radiation diffraction is also performed.

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References and links

1. Introduction
Lamellar Multilayer Gratings (LMG) offer increased spectral and angular resolution in the soft x-ray (SXR) region compared to conventional multilayer mirrors (MM). The resolution of MMs in the SXR region is inherently limited due to absorption [1]. By fabricating a grating
structure into a MM, an LMG structure is obtained that allows the SXR to penetrate deeper into the multilayer stack. Effectively, more bi-layers contribute to the reflection, improving the spectral and angular resolution of the MM. A schematic representation of an LMG is shown in Fig. 1 and more detailed descriptions of the working principles of LMGs can be found in Refs. [2–7].

Till now, diffraction of SXR from LMGs has been analyzed by time-consuming numerical simulations using complex rigorous theories [2,7,8]. Generally, one would not expect that computation time would be a significant limitation when addressing a physical problem. However, the optimization of LMG performance, in terms of resolution and reflectivity, is very difficult, as many of these time-consuming simulations need to be performed. It is even more difficult for the inverse problem of obtaining multilayer structural data, such as intermixing or roughness, from reflectivity measurements. Here, a multi-dimensional fitting procedure needs to be performed requiring hundreds or even thousands of simulations. Computation time is, thus, an important aspect when trying to understand the optical properties of LMGs. The lack of easy optimization and difficulties in understanding the LMG physical structure hampers the implementation of these dispersive elements in the SXR region.

Some progress in reducing computation time has recently been made in Ref. [6], where we used a coupled-waves approach (CWA). Additionally, we identified a single-order operating regime. In this regime, the incident wave only excites one diffraction order and, hence, the problem of diffraction is simplified as a two-wave approximation can be used. Nevertheless, the approach described in this work still requires numerical calculations [6].

In this paper, we will derive analytic expressions for the diffraction efficiency of SXR radiation by LMGs operating in the single-order regime. We will demonstrate that these expressions are in excellent agreement with results from rigorous diffraction theories. This analytical description of the optical properties of LMGs makes earlier, complex, theories redundant. Furthermore, this theory can be used to improve our understanding of the optical properties of LMGs, simplify their design and optimization, and, most importantly, reveal their ultimate potential performance.

In section 2, we will first describe the differential equations of the CWA that can be rigorously used to calculate LMG SXR diffraction efficiency with numerical methods. Next, in section 3, we will derive the analytical solution to these differential equations for the zero-order diffraction efficiency (reflectivity) for LMGs operating in single-order regime. We will compare the reflectivity obtained using our analytic solution to that obtained from rigorous diffraction theory and demonstrate excellent agreement between them. In section 4, the analytical solution for the diffraction efficiency of higher diffraction orders is derived and discussed. Again, we will show an excellent agreement between rigorous diffraction theory and our simple analytical expressions. Finally, in section 5, a concise discussion of the diffraction of p-polarized radiation by LMGs will be presented.

2. Differential equations of the coupled waves approach

A comprehensive description of a CWA used to calculate diffraction and reflection by LMGs is given in Ref. [6]. Certain parts of that description are repeated here, as they are required for our derivation of analytical expressions. We begin with a schematic representation of an LMG as shown in Fig. 1(a). Here, a two-component (absorber A and spacer S) periodic multilayer structure with bi-layer period $d$ and thickness ratio $\gamma$ is depicted. The Z-axis is defined as directed into the depth of the substrate and $L$ is the total thickness of the multilayer structure. The spatial distribution of the dielectric permittivity $\varepsilon$ and the piece-wise periodic function $U$ can be written as
A surface relief grating (SG) with period and lamellar width 

Fig. 1. Schematic of the cross section of an LMG. (a): An incident beam from the left (In), under grazing angle \(\theta_0\), is reflected from the multilayer and diffracted into multiple orders (Out) by the grating structure. The multilayer is built up from \(N\) bi-layers with thickness \(d\). Each bi-layer consists of an absorber material (A) with thickness \(\gamma d\) and a spacer material (S) with thickness \((1-\gamma)d\). The grating structure of the LMG is defined by the grating period \(D\) and lamellar width \(\Gamma D\). (b): The normalized function \(U(x)\) is used to describe the lamellar profile.

Where \(\chi = 1-\varepsilon\) is the polarizability of matter. The piece-wise periodic function \(U\), shown in Fig. 1(b), describes the lamellar profile in the X-direction and can be expanded into a Fourier series:

The solution to the 2D-wave equation \(\nabla^2 E(x,z) + k^2 \varepsilon(x,z)E(x,z) = 0\) then has the following form (chapter 1, Ref. [9]):

where \(\delta_{n,0}\) is the Kronecker symbol, and \(\kappa_n = \sqrt{k^2 - q_n^2}\) and \(\kappa_n^{(z)} = \sqrt{k^2 \varepsilon_{sub} - q_n^2}\) are the Z-components of the wave vector for the \(n^{th}\) diffraction order in vacuum and in the substrate, respectively. The boundary conditions in Eqs. (4) signify that only a single plane wave is incident on the LMG at the grazing angle \(\theta_0\), and that there are no waves incident onto the LMG from the substrate.
Still following the derivation of Ref. [6], let us now represent the field of the \( n \)th order diffracted wave \( F_n(z) \) as a superposition of two waves propagating in opposite directions along Z-axis:

\[
F_n(z) = A_n(z)\exp(ik_nz) + C_n(z)\exp(-ik_nz)
\]

For a unique determination of the functions \( A_n(z) \) and \( C_n(z) \) we impose an additional requirement:

\[
A'_n(z)\exp(ik_nz) + C'_n(z)\exp(-ik_nz) = 0
\]

where the prime symbol in \( A'_n \) and \( C'_n \) indicates a first derivative with respect to \( z \).

The functions \( A_n(z) \) and \( C_n(z) \) can be considered as amplitudes of a transmitted and a reflected wave, respectively. The representation of the diffracted waves in the form of Eqs. (5) and (6) is especially useful for the x-ray and soft x-ray region, because the polarizability of all materials \( (\varepsilon = 1 - \chi) \) is very small. This small polarizability means that the Z-component of the wave vector in vacuum

\[
k_n = \sqrt{k^2 - q_n^2}
\]

is very close to that in matter \( \kappa_n(z) = \sqrt{k^2\varepsilon - q_n^2} \). As a result, the amplitudes \( A_n(z) \) and \( C_n(z) \) vary slowly with \( z \) compared with the quickly oscillating exponential multipliers as long as the angle of incidence does not satisfy total external reflection.

By substituting Eqs. (5) and (6) into Eqs. (4) we obtain a system of first order differential equations for the amplitudes \( A_n(z) \) and \( C_n(z) \)

\[
\begin{align*}
\frac{dA_n(z)}{dz} &= -\frac{ik^2}{2\kappa_n} \chi(z) \sum_{m=-\infty}^{\infty} U_{n,m} \left[ A_m(z)e^{i(k_m-k_n)z} + C_m(z)e^{-i(k_m+k_n)z} \right] \\
\frac{dC_n(z)}{dz} &= +\frac{ik^2}{2\kappa_n} \chi(z) \sum_{m=-\infty}^{\infty} U_{n,m} \left[ A_m(z)e^{i(k_m+k_n)z} + C_m(z)e^{-i(k_m-k_n)z} \right]
\end{align*}
\]

with the following boundary conditions

\[
A_n(0) = \delta_{n,0} ; \quad C_n(L) = 0
\]

The dielectric permeability of the substrate is set to unity in Eq. (8), which is quite reasonable for soft x-rays as the polarizability is very small. We can, therefore, neglect the effect of reflection and diffraction of the incident wave from the substrate. Evidently, diffraction and reflection from an LMG can be determined by numerically solving Eqs. (7) and (8) and calculating the amplitudes of the waves diffracted into the vacuum \( (r_n = C_n(0)) \) and substrate \( (t_n = A_n(L)) \).

In Ref. [6], we have already compared numerical simulations using Eqs. (7) and (8) to calculations performed by other authors [7] and found excellent agreement provided sufficient diffraction orders are taken into account. In that work, we also identified a single-order operating regime for LMGs in which, an incident plane wave can only excite a single diffraction order. It was shown that, in this regime, the LMG zeroth-order diffraction efficiency (reflectivity) can be calculated by replacing the LMG by a conventional multilayer mirror (MM) with its material densities reduced by a factor of \( \Gamma \) (the ratio of the lamell width to grating period). The angular width of the zeroth-order diffraction peak of an LMG then simply reduces by a factor of \( 1/\Gamma \) without loss of peak reflectivity compared to a conventional MM. The necessary condition for LMG operation in the single-order regime is quite evident: the angular width of the LMG Bragg peak \( \Gamma \Delta \theta_{BM} \) (where \( \Delta \theta_{BM} \) is the Bragg peak width for
conventional MM) should be small compared with the angular distance between neighboring
diffraction peaks \(d/D\), such that [6]:

\[
\Gamma D \Delta \theta_{mm} \ll d
\]  

(9)

3. Analytical solution for the zeroth-order diffraction efficiency (reflectivity)

In the previous section, we briefly discussed the most important aspects of the differential
equations used in the coupled-waves approach as applicable to the LMG single-order regime
[6]. From these differential equations, we will now derive analytical expressions for the
diffraction efficiency of s-polarized SXR radiation by LMGs in single-order operation. In the
single-order regime, all higher diffraction orders in Eqs. (7) can be neglected, leaving only the
incident and specularly reflected waves

\[
\begin{align*}
\frac{dA_{0}(z)}{dz} & = -\frac{ik^{2}}{2\kappa_{0}} \Gamma \chi(z) \left[ A_{0}(z) + C_{0}(z) \cdot e^{-2i\kappa_{0}z} \right] \\
\frac{dC_{0}(z)}{dz} & = +\frac{ik^{2}}{2\kappa_{0}} \Gamma \chi(z) \left[ A_{0}(z) \cdot e^{2i\kappa_{0}z} + C_{0}(z) \right]
\end{align*}
\]  

(10)

where \(A_{0}(0) = 1\) and \(C_{0}(L) = 0\). One can see that Eqs. (10) coincide with those describing the
reflectivity of a conventional MM, except for the factor \(\Gamma\) that has appeared as a multiplier in
front of the polarizability. As the polarizability in the SXR region is directly proportional to
the material density, we can conclude that Eqs. (10) describe the reflection of an SXR wave
from a conventional multilayer structure with the material density scaled by \(\Gamma\), as was also
found in Ref. [6].

Let us now consider a periodic multilayer structure having abrupt interfaces and consisting
of two materials, namely a spacer and an absorber, with polarizabilities \(\chi_{s}\) and \(\chi_{a}\),
respectively. Then

\[
\chi(z) = \chi_{s} + (\chi_{a} - \chi_{s}) \cdot u(z)
\]  

(11)

describes the modulation of the multilayer and the piece-wise function \(u\) is similar to the
function \(U\) that describes the lamellar profile:

\[
u(z; \gamma, d) = \sum_{n=-\infty}^{\infty} u_{n} \exp \left( \frac{2i\pi n z}{d} \right), \quad u_{n} = \gamma, \quad u_{n=0} = \frac{1}{2i\pi n} \left[ 1 - \exp(-2i\pi n \gamma) \right]
\]  

(12)

We limit ourselves to the most important case of a wave incident onto the multilayer structure
within or near the Bragg resonance of the \(j\)th order, i.e. we will suppose that \(j \lambda \approx 2d \sin \theta_{0}\) or,
equivalently, \(\kappa_{0} \approx \pi j / d\). Substituting Eqs. (11) and (12) into Eqs. (9) we obtain

\[
\begin{align*}
\frac{dA_{0}(z)}{dz} + \frac{ik^{2}}{2\kappa_{0}} \left[ \bar{\chi} \Gamma A_{0}(z) + (\chi_{a} - \chi_{s}) u_{j} \Gamma C_{0}(z) \cdot e^{2i(\pi j / d - \kappa_{0}z)} \right] & = \Delta A(z) \\
\frac{dC_{0}(z)}{dz} - \frac{ik^{2}}{2\kappa_{0}} \left[ \bar{\chi} \Gamma C_{0}(z) + (\chi_{a} - \chi_{s}) u_{-j} \Gamma A_{0}(z) \cdot e^{-2i(\pi j / d - \kappa_{0}z)} \right] & = \Delta C(z)
\end{align*}
\]  

(13)

where \(\bar{\chi} = \chi_{a} \gamma + \chi_{s} (1 - \gamma)\) is the mean polarizability of a multilayer structure. The left-hand
side of Eqs. (13) contain all terms that vary slowly with \(z\). The functions \(\Delta A\) and \(\Delta C\) on the
right-hand side denotes all other terms that oscillate quickly with \(z\). These only weakly
influence the amplitudes \(A_{0}\) and \(C_{0}\) and, therefore, can be neglected. Formally, this can be
expressed by averaging Eqs. (13) over an interval, \(\Delta z\), that is substantially larger than the
period of oscillations of the functions $\Delta A$ and $\Delta C$, but much smaller than the typical length scale over which the functions $A_0$ and $C_0$ vary.

A system of coupled differential equations with constant coefficients can be obtained by introducing $a_0(z) = A_0(z) \cdot \exp[-i(\pi j / d - \kappa_0)z]$ and $c_0(z) = C_0(z) \cdot \exp[i(\pi j / d - \kappa_0)z]$:

$$
\begin{align*}
\frac{da_0(z)}{dz} + i \left( \frac{\pi j}{d} - \kappa_0 + \frac{k^2}{2\kappa_0} \right) a_0(z) + i \frac{k^2}{2\kappa_0} (\chi_A - \chi_S) \Gamma u_j c_0(z) &= 0 \\
\frac{dc_0(z)}{dz} - i \left( \frac{\pi j}{d} - \kappa_0 + \frac{k^2}{2\kappa_0} \right) c_0(z) - i \frac{k^2}{2\kappa_0} (\chi_A - \chi_S) \Gamma u_j a_0(z) &= 0
\end{align*}
$$

with the same boundary conditions $a_0(0) = 1$ and $c_0(L) = 0$ as for Eqs. (10). By solving Eqs. (14) we obtain an analytical expression for the zeroth-order diffraction efficiency

$$
R_0 = \left| \frac{B \tanh(SNd)}{b \tanh(SNd) - i\sqrt{B_+ B_- b^2}} \right|^2
$$

(15)

where $R_0 = |\eta_1|$. The terms used in Eq. (15) are

$$
b = \chi \Gamma + 2 \sin \theta_0 \left( \frac{\lambda}{2d} - \sin \theta_0 \right) ; \quad B_+ = (\chi_A - \chi_S) u_j \Gamma ; \quad S = \frac{k}{2\sin \theta_0} \sqrt{B_+ B_- b^2}
$$

(16)

where the Bragg parameter, $b$, characterizes a deviation from the Bragg resonance, the parameters $B_+$ describe the modulation of the structure, and the parameter $S$ characterizes the variation of the amplitudes $A_0$ and $C_0$ with $z$. The number $N$ is the total number of bi-layers in the multilayer structure.

Vinogradov and Zeldovich have previously derived Eq. (15) in Refs. [10,11]. However, they used a somewhat different mathematical technique and, in contrast to our approach, neglected the second derivatives with respect to $z$ of the slowly varying amplitudes. As a result, there is a small difference in the expression for the Bragg parameter $b$.

To demonstrate the effect of the different Bragg parameters, $b$, Fig. 2 shows calculated reflectivities versus the grazing incidence angle using 3 different approaches. These calculations were performed for a conventional Mo/B$_4$C multilayer mirror (i.e. for $\Gamma = 1$) at $E = 183.4$eV, which is the characteristic boron K\textsubscript{$\alpha$}-line. Curve 1 is the result of exact calculations using a recurrent algorithm [12], while curve 2 was calculated via Eqs. (15) and (16). Curve 3 was calculated using the Bragg parameter derived by Vinogradov and Zeldovich. It can easily be seen that curves 1 and 2 are in better agreement outside the Bragg peak than curves 1 and 3. Figure (2), thus, demonstrates that the Bragg parameter, $b$, deduced above (Eq. (16)) is better suited for the calculation of MM reflectivity than the parameter deduced by Vinogradov and Zeldovich.

We will now continue our investigation by deriving the generalized Bragg condition for LMGs. For simplicity, we begin by assuming a semi-infinite multilayer structure ($N \to \infty$). Equation (15) then reduces to its simplest form with $\tanh(SNd) = 1$. The Bragg peak is very narrow, because of the small polarizability of matter in the SXR wavelength region. Therefore, we can neglect the wavelength dependence of the dielectric constant inside the peak. The reflectivity then only depends on the incidence angle and the radiation wavelength through the Bragg parameter $b$. At maximum reflectivity, we have the condition $dR_0 / d\tau = 2 \text{Re} \left[ r^* \left( dr / db \right) \left( db / d\tau \right) \right] = 0$ (where either $\tau = \sin \theta_0$ or $\tau = \lambda$) and we can obtain a Bragg condition that also includes the absorption and refraction of radiation.
Fig. 2. Reflectivity $R_0$ (at $E = 183.4$ eV) of conventional Mo/B$_4$C multilayer mirror ($d = 6$ nm, $\gamma = 0.34$, $N = 50$) versus grazing angle. Calculations were performed with the use of exact algorithm (curve 1, red), simple analytic expressions (15) and (16) deduced in the present paper (curve 2, blue), and formulas obtained in Ref. [10,11]. (curve 3, green).

$$\frac{j \lambda}{2d} = \sin \theta_b - \frac{\Gamma}{2 \sin \theta_b} \left[ \text{Re} \, \zeta - \text{Re}(\chi_a - \chi_s) \cdot \frac{\text{Im}(\chi_a - \chi_s)}{\text{Im} \, \zeta} \cdot \frac{\sin^2(\pi j \gamma)}{(\pi j)^2} \right]$$ \hspace{1cm} (17)

If the Bragg condition (Eq. (17)) is fulfilled, the reflectivity achieves a peak value, which can be written in a very simple manner [1]

$$R_{\text{peak}} = \frac{1 - w}{1 + w}; \quad w = \sqrt{\frac{1 - y^2}{1 + f^2 y^2}}; \quad f = \frac{\text{Re}(\chi_a - \chi_s)}{\text{Im}(\chi_a - \chi_s)}; \quad y = \frac{\text{Im}(\chi_a - \chi_s)}{\text{Im} \, \zeta} \cdot \frac{\sin(\pi j \gamma)}{\pi j}$$ \hspace{1cm} (18)

From Eq. (18), it can be seen that the peak reflectivity is independent of the grating parameters and corresponds to that of a conventional multilayer mirror [1]. This is because the parameters $f$ and $y$ determine the peak reflectivity entirely and these parameters are not changed if the density of both materials is scaled by the same factor, $\Gamma$. In contrast, the penetration depth of the radiation into the multilayer structure $L_{MS}$, and therefore also the spectral and angular resolution of an LMG, is inversely proportional to $\Gamma$:

$$L_{MS} \sim \frac{1}{S} = \frac{\lambda \sin \theta_b}{\pi \Gamma \text{Im} \, \zeta \cdot \sqrt{(1 - y^2)(1 + f^2 y^2)}}$$ \hspace{1cm} (19)

LMGs can, thus, offer improved resolution without loss of peak reflectivity. Note that the peak reflectivity, (Eq. (18)), chieves its maximum possible value when the parameter $y$ is maximal and, hence, the thickness ratio, $\gamma$, of a multilayer structure obeys the equation

$$\tan(\pi j \gamma) = \pi j \left[ y + \text{Im} \, \chi_s / \text{Im}(\chi_a - \chi_s) \right]$$ \hspace{1cm} (20)

which is well-known in the theory of conventional SXR multilayer mirrors [10,11].

Figure 3 demonstrates the accuracy of the analytic expressions (15) and (16) for the reflectivity of LMGs operating in the single-order regime. For these calculations, the lamellar width $\Gamma D = 70$ nm was fixed, while the parameter $\Gamma$ and the grating period $D$ were varied. The number of bi-layers $N$ was chosen to be large enough to provide the maximum possible peak reflectivity. The colored curves were calculated using rigorous diffraction theory, as described.
by Eqs. (7), where 5 diffraction orders were taken into account. The black dashed curves were calculated using the analytic Eq. (15). Figure 3 shows that the agreement between the curves is excellent with a deviation in reflectivity peaks of less than 0.6%. In addition, it can be seen that the width of the Bragg peak decreases proportionally to $\Gamma$ and that the peak reflectivity of the LMG corresponds to that of a conventional MM. The shift in the peak position is caused by the dependence on the $\Gamma$-ratio of the Bragg condition (Eq. (17)) as the “effective” polarizabilities of both materials are scaled by this factor. Here, the “effective” polarizability refers to the average polarizability of an individual layer.

Fig. 3. Reflectivity (at $E = 183.4$ eV) versus the grazing angle of an incident beam for a conventional Mo/B₄C multilayer mirror ($\Gamma = 1$) and for LMGs with different $\Gamma$-ratios: $\Gamma = 1/2$, $1/3$, and $1/10$. The multilayer parameters are the same as for Fig. 2, with the exception that the number of bi-layers increases with $\Gamma$ according to $N = 100/\Gamma$. The lamel width $D$ is fixed at 70nm and so the grating period increases through the relation $D = 70 \text{ nm} / \Gamma$. The colored curves were calculated with the use of rigorous coupled waves approach (Eq. (7)), where 5 diffraction orders were taken into account, while black dashed curves were calculated via simple analytic expressions (Eqs. (15) and (16)).

4. Analytic solution for higher-order diffraction efficiencies

In the previous section, we derived analytical expressions for the specular reflection of an LMG where it is, essentially, used as a mirror. This is because the diffraction angle of all orders except the zeroth order falls into an angular range where the multilayer shows no noticeable reflection. A more correct term would, thus, actually be Lamellar Multilayer Mirror (LMM). However, an LMG can also be used as a conventional diffraction grating, decomposing incident radiation of a single direction into diffracted light where the emission angle depends on the wavelength. Let us now consider the $m^{th}$ order diffraction efficiency, where we limit the analysis to angles and wavelengths close to the Bragg resonance (quasi-Bragg resonance), i.e. assuming $j \lambda \approx d (\sin \theta_i + \sin \theta_m)$ or, equivalently, $\kappa_r + \kappa_m \approx 2 \pi j / d$. Here, the index, $j$, is the order of the Bragg reflection from a multilayer structure, and the index, $m$, is the order of diffraction from the grating surface. Quasi-Bragg resonance means that there is constructive interference of waves diffracted from different interfaces of the multilayer structure and, hence, a high diffraction efficiency. In addition, the LMG will be limited to the single order regime.

One can check directly from Eqs. (7) that the amplitudes $A_j(z)$ and $C_m(z)$ only interrelate resonantly with each other, and we can therefore neglect all other equations in the
CWA system (Eqs. (7)). Then, similar to the previous section, we introduce
\[ a_n(z) = A_n(z) \exp \left[ -i \left( \frac{\pi j}{d} - \frac{\kappa_n + \kappa_m}{2} \right) z \right] \]
and
\[ c_n(z) = C_n(z) \exp \left[ i \left( \frac{\pi j}{d} - \frac{\kappa_n + \kappa_m}{2} \right) z \right], \]
and obtain a system of differential equations with constant coefficients:
\[ \begin{align*}
\frac{da_n(z)}{dz} + i \left( \frac{\pi j}{d} - \frac{\kappa_n + \kappa_m}{2} + \frac{k^2}{2\kappa_n} \right) a_n(z) + i \frac{k^2}{2\kappa_n} (\chi_n - \chi_m) u_{n-1} c_n(z) &= 0 \\
\frac{dc_n(z)}{dz} - i \left( \frac{\pi j}{d} - \frac{\kappa_n + \kappa_m}{2} + \frac{k^2}{2\kappa_m} \right) c_n(z) - i \frac{k^2}{2\kappa_m} (\chi_n - \chi_m) u_{n+1} a_n(z) &= 0
\end{align*} \tag{21} \]
Solving Eqs. (21), one finds an expression for the diffraction efficiency \( R_n = |r_n|^2 \Re \kappa_n / \kappa_0 \),
which has the same form as Eq. (15). However, the parameters \( B, b, \) and \( S \) are somewhat different to those in Eqs. (16):
\[ \begin{align*}
B &= (\chi_n - \chi_m) u_{n+1} U_{n-1} ; \\
S &= \frac{k}{2 \sin \theta_0 \sin \theta_m} \sqrt{B_0 B - b^2} ; \\
b &= \frac{\sin \theta_0 + \sin \theta_m}{2 \sqrt{\sin \theta_0 \sin \theta_m}} \Gamma + 2 \sqrt{\sin \theta_0 \sin \theta_m} \left( \frac{j \lambda}{2d} - \frac{\sin \theta_0 + \sin \theta_m}{2} \right)
\end{align*} \tag{22} \]
Please note that the diffraction angle, \( \theta_m \), is not an independent variable but depends on the
grazing angle of the incident beam \( \theta_0 \) through the grating equation \( \cos \theta_m = \cos \theta_0 + m\lambda / D \).

Similar to Eq. (17), the generalized Bragg condition can be written as
\[ \frac{j \lambda}{2d} - \frac{\sin \theta_0 + \sin \theta_m}{2} \sin \theta_0 + \sin \theta_m \Re \frac{\chi_n - \chi_m}{\sin \theta_0 + \sin \theta_m} \Gamma + \frac{\Re (\chi_n - \chi_m)}{\sin \theta_0 + \sin \theta_m} \Im \frac{\chi_n - \chi_m}{\sin \theta_0 + \sin \theta_m} \sin^2(\pi j) \sin^2(\pi m \Gamma) \tag{23} \]
The peak value of the diffraction efficiency then has the same form as in Eq. (18), but the parameter \( y \) is more complex:
\[ y = \frac{\Im (\chi_n - \chi_m)}{\Im \frac{\chi_n - \chi_m}{\sin \theta_0 + \sin \theta_m} \sin(\pi j) \sin^2(\pi m \Gamma)} \frac{2 \sqrt{\sin \theta_0 \sin \theta_m}}{\pi j} \sin(\pi m \Gamma) \tag{24} \]
As a quick check of these equations, one would expect that, for specular reflectivity [i.e. inserting \( m = 0 \) into Eqs. (21)–(24)], we should obtain Eqs. (14)–(17), which is indeed the case.

To investigate the accuracy of the expressions (15) and (22), we compared results deduced from these equations with those obtained using rigorous diffraction theory (Eqs. (7)). As an example of such a comparison, Fig. 4 shows the zeroth to −5th order diffraction peaks as a function of the grazing angle of the incident beam. The colored curves were numerically calculated using rigorous diffraction theory, where 9 diffraction orders, from + 2nd to −6th order, were taken into account. The black dashed curves were calculated using the analytic expressions (15) and (22). The parameters of the multilayer structure were the same as for Fig. 3. The grating period \( D \) was 210 nm, the lamellar width \( \Gamma D \) was 70 nm and the number of bi-layers \( N \) was 300. As can be seen, the agreement between the curves is excellent with less than 0.6% deviation in diffraction peaks, except for the very small −3rd order diffraction peak. A closer look at the −3rd order diffraction peak shows that our parameter choices (specifically
Gamma = 1/3) yields $B_{\Gamma} = 0$. Under these circumstances, the small residual reflection comes from the quickly oscillating terms, which are neglected in the derivation of the analytical solution (Eq. (21)). From these observations it can be concluded that these extremely small peaks can be neglected in practical applications. Hence, as was found for the reflectivity calculations, complicated rigorous diffraction theories are not required for the calculation of the diffraction efficiencies of LMGs operating in the single order regime.

![Graph](https://via.placeholder.com/150)

Fig. 4. Diffraction efficiency $R_n$ (for $n = -5,...,0$) at $E = 183.4$ eV versus grazing angle of the incident beam. Parameters of the LMG: Mo/B$_4$C multilayer structure ($d = 6$ nm, $\gamma = 0.34$, $N = 300$), $D = 210$ nm, $\Gamma = 1/3$. The colored curves were calculated using the rigorous coupled waves approach, where 9 diffraction orders (from +2nd to −6th) were taken into account. The black dashed curves were calculated via the simple analytical expressions (15) and (22). The agreement is excellent, except for the −3rd order (blue curve).

While the expressions for the reflectivity and the higher-order diffraction efficiencies are very similar, they differ in certain details. The main difference is the dependence of the maximum diffraction efficiency on the $\Gamma$-ratio in Eq. (24) for the parameter $\gamma$. The diffraction efficiency becomes higher for larger values of $\gamma$. However, the $\Gamma$-ratio is always smaller than unity for a grating, so each multiplier in Eq. (24) is also less than unity, and the parameter $\gamma$ for the higher order diffraction efficiencies is always less than that of the zeroth order diffraction efficiency (Eq. (18)). Hence, the peak value of the higher order diffraction efficiencies, $R_n$, will increase with decreasing $\Gamma$, but not exceed the reflectivity peak value $R_0$. Note that the parameter $\gamma$ providing the maximum of diffraction efficiency is the same as for the reflectivity and is determined by Eq. (20).

In Fig. 5, the $\Gamma$-dependence of higher order diffraction efficiencies is demonstrated by showing the −1st order diffraction efficiencies for different values of $\Gamma$. The parameters of the multilayer structure are the same as for Figs. 3 and 4. The lamellar width $\Gamma D = 70$ nm is fixed, while $\Gamma$ and the grating period, $D$, are varied. The number of bi-layers $N$ is again chosen large enough (100/$\Gamma$) to obtain the maximum possible diffraction efficiency. The colored curves were calculated on the basis of rigorous diffraction theory (where 5 diffraction orders were taken into account) and black curves were calculated with the use of the analytical Eqs. (15) and (22). The agreement between the curves is excellent for all values of $\Gamma$. By comparing Figs. 4 and 5, it can be seen that the −1st order diffraction efficiency is almost as high as the reflectivity, with a relative difference of only 0.85% for $\Gamma = 1/20$. 

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5. Diffraction of p-polarized radiation by LMG

In the previous sections we have considered diffraction and reflection of s-polarized radiation by LMGs. In this section, we will discuss diffraction and reflection of p-polarized radiation. For p-polarized radiation, a slightly different expression for the dielectric constant distribution in the LMG is required. In accordance with Eqs. (1) and (12), the distribution of the dielectric constant inside an LMG (0 < z < L) can be written as the 2D Fourier series

$$\epsilon(x, z) = 1 - \frac{\Gamma}{\pi} \sum_m U_m e^{i \pi m D / \Gamma} \left( \chi_A - \chi_S \right) \cdot \sum_{m} \sum_{j=0} U_m U_j e^{i \pi (mD + jz)} (25)$$

The single-order regime is characterized by a suitable choice of parameters such that one only needs to keep the term with $m = 0$ in the first sum and only one harmonic with fixed $m$ and $j$ in the second sum. The first term, $\frac{\Gamma}{\pi}$, describes the propagation of an incident wave through an LMG neglecting reflection and diffraction and the second term gives the main contribution to the reflectivity or diffraction efficiency under Bragg or quasi-Bragg resonance $j\lambda \approx d(\sin \theta_0 + \sin \theta_m)$. In other words, to solve the wave equation in the single-order regime, it is sufficient to use (instead of Eq. (25))

$$\epsilon(x, z) \approx 1 - \frac{\Gamma}{\pi} \left( \chi_A - \chi_S \right) U_m U_j e^{i \pi (mD + jz) / \Gamma} (26)$$

Here we will now analyze the diffraction and reflection of p-polarized radiation as well. However, the corresponding 2D wave equation is more involved due to the presence of first derivatives $\nabla^2 H + k^2 \epsilon H - \nabla(\ln \epsilon) \cdot \nabla H = 0$ where $H$ is the nonzero Y-component of the magnetic field perpendicular to the plane of Fig. 1 and where $\nabla \equiv \frac{\partial}{\partial x} + i \frac{\partial}{\partial z}$. To simplify the wave equation, we introduce a new field function $\tilde{H}(x, z) = H(x, z) / \sqrt{\epsilon(x, z)}$, which obeys the 2D-wave equation without the first derivatives of the field.
\( \nabla^2 \hat{H}(x, z) + k^2 \bar{\varepsilon}(x, z) \hat{H}(x, z) = 0 \), achieved by introducing a modified function \( \bar{\varepsilon}(x, z) \). It can be shown that \( \bar{\varepsilon}(x, z) \) relates to the original dielectric function as follows

\[
\bar{\varepsilon}(x, z) \equiv \varepsilon(x, z) + \frac{1}{2k^2} \nabla^2 \varepsilon(x, z) - \frac{3}{4k^2} \left( \nabla \varepsilon(x, z) \right)^2 \quad (27)
\]

Expanding Eq. (27) into a 2D Fourier series and keeping only linear terms, justified by the small polarizabilities \( \chi_S \) and \( \chi_A \), we obtain, instead of Eq. (25)

\[
\bar{\varepsilon}(x, z) = 1 - \bar{\chi} \sum_m U_m e^{2\pi imx/D} \left[ 1 - \frac{1}{2} \left( \frac{m\lambda}{D} \right)^2 \right] - \\
(\chi_A - \chi_S) \sum_m \sum_{j=0} U_m U_j e^{2\pi (m\lambda + j\lambda)/d} \left[ 1 - \frac{1}{2} \left( \frac{j\lambda}{d} \right)^2 - \frac{1}{2} \left( \frac{m\lambda}{D} \right)^2 \right] \quad (28)
\]

As before, we are interested in reflection and diffraction by LMGs operating in the single-order regime near the Bragg or quasi-Bragg resonance. Keeping only specific terms in Eq. (28) we obtain

\[
\varepsilon(x, z) \approx 1 - \bar{\chi} \left( \chi_A - \chi_S \right) U_m U_j e^{2\pi (m\lambda + j\lambda)/d} \left[ 1 - \frac{1}{2} \left( \frac{j\lambda}{d} \right)^2 - \frac{1}{2} \left( \frac{m\lambda}{D} \right)^2 \right] \approx 0 \quad (29)
\]

Here, the resonance condition of diffraction \( j\lambda/d \approx \sin \theta_0 \pm \sin \theta_m \) and the grating equation \( m\lambda/D = \cos \theta_m - \cos \theta_0 \) were taken into account. Equation (29), which is valid for p-polarized light, can now be compared with the expression for s-polarized light (Eq. (26)). The comparison shows that all the expressions deduced above for s-polarized radiation are also valid for p-polarized radiation, if we replace the dielectric modulation of the multilayer structure \( \chi_A - \chi_S \) by \( (\chi_A - \chi_S) \cos(\theta_0 + \theta_m) \). This proves that, independent of the polarization, an analytical calculation of reflection and diffraction by LMGs is possible.

Equation (29) clearly demonstrates the main feature of p-polarized radiation reflection, namely, that at Brewster's angle of incidence \( \theta_0 = \pi / 4 \), the modulation effect of a multilayer structure disappears and the reflectivity (the zeroth order diffraction efficiency) goes to zero. Similarly, the \( m^{th} \) order diffraction efficiency goes to zero if the diffracted beam propagates perpendicular to the incident one, i.e. at \( \theta_0 + \theta_m = \pi / 2 \).

6. Conclusions

We developed an analytical theory for the reflection and diffraction of soft x-rays (SXR) by Lamellar Multilayer Gratings (LMGs) operating in the single-order regime. In this regime, an incident plane wave can only excite a single diffracted plane wave. The description of diffraction then becomes much easier, because a two-wave approximation can be used. Being mostly interested in cases of practical importance at or near the Bragg or quasi-Bragg resonance, we deduced simple analytical expressions describing the reflection and diffraction efficiencies as function of incidence angle and radiation wavelength.

Analytical expressions for diffraction efficiencies were first derived for LMGs in specular reflectance, i.e. expressions for the zeroth-order diffraction efficiency (reflectivity). The resolution of an LMG (angular width of the Bragg peak) was shown to grow inversely with the \( \Gamma \)-ratio (ratio of lamel width to grating period), provided that the number of bi-layers
increases inversely proportional to \( \Gamma \). At the same time, the peak value of the reflectivity is independent of the grating parameters and can be as high as that of a conventional MM. It was also shown that the reflectivity peak of a single-order LMG is the same as that of a conventional MM for which the material densities have been reduced by a factor of \( \Gamma \). Therefore, the choice of optimal parameters for the multilayer structure (composition and \( \gamma \)-ratio) remains the same. However, in contrast to a conventional MM, the resolution of an LMG is not limited by the absorption of radiation and is independent of the peak reflectivity. LMGs can therefore be considered as MMs with no physical limitation on their resolution and without loss of peak reflectivity. However, resolution and reflectivity are still limited by the structures that can be fabricated. The analytical approach, thus, confirmed the main results of Ref. [6], where the rigorous coupled-waves approach was numerically solved.

Expressions describing diffraction efficiencies and peak efficiencies for higher orders have been deduced. These results are very similar to those for the zeroth order reflection, differing only in certain details. The main difference is the dependence of the diffraction efficiency on the \( \Gamma \)-ratio: for smaller \( \Gamma \)-ratios, the peak diffraction efficiency approaches, but does not exceed, the peak reflectivity. Also, a decreasing \( \Gamma \) results in a narrowing of the diffraction peak in terms of grazing angle of the incident radiation. The parameters of the multilayer structure (composition and \( \gamma \)-ratio) providing maximum diffraction efficiency proved to be the same as for the reflectivity maximum.

The analytical expressions describing diffraction and reflection of LMGs were demonstrated to be in excellent agreement with those obtained using the rigorous coupled-waves approach. We, therefore, conclude that, in the single-order regime, complex and time-consuming computer codes, based on rigorous theories, are not required for the calculation of the reflection and diffraction by LMGs. Optimization of LMG parameters or deducing structural information, such as intermixing or roughness, of the LMG multilayer from reflectivity measurements are, thus, significantly simplified. This opens several opportunities for the investigation of the fabrication and use of LMGs in the SXR wavelength region.

We also analyzed diffraction and reflection of \( p \)-polarized radiation and showed that LMGs can be described analytically for \( p \)-polarized radiation as well, in an analogous manner that found for \( s \)-polarized radiation. The only difference compared to \( s \)-polarized radiation is a reduced efficiency of reflection and diffraction at Brewster’s angle of incidence, i.e. when the reflected or diffracted beam propagates perpendicular to the incident one.

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