Extended theory of soft x-ray reflection for realistic lamellar multilayer gratings

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Abstract: An extended set of coupled wave equations were derived to describe non-idealized lamellar multilayer grating structures with properties as obtained with state-of-the-art fabrication techniques. These generalized equations can include all relevant effects describing the influence of passivation and contamination layers, non-rectangular lamel profiles and sidewall scalloping. The calculations showed that passivation and contamination plays an important role in that it may significantly reduce peak reflectivity. However, we also derived a condition for layer thicknesses having negligible effects. Slightly positive tapered lamel profiles are shown to further reduce the bandwidth as compared to a rectangular lamel profile, whereas negative tapers significantly increased the bandwidth. The influence of intriguing effects, such as the sidewall scalloping caused by Bosch Deep Reactive Ion Etching, are also modeled. We identified the signature of such scalloping as additional side peaks in the reflectivity spectrum and present parameters with which these can be effectively suppressed.

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1. Introduction

Lamellar multilayer gratings (LMG) are a newly emerging component for the EUV and soft x-ray (SXR) spectral ranges. They effectively suppress the detrimental influence of absorption, which limits the resolution of conventional multilayer (ML) mirrors, through the fabrication of a grating structure in such a ML mirror. Such LMGs show potential for use in applications where soft x-rays need to be filtered or monochromatized. An important example is x-ray fluorescence analysis, where an increase in spectral resolution $E/\Delta E$ of the analyzer, e.g. a Bragg crystal or ML mirror, results in an improvement of chemical specificity and sensitivity. A schematic representation of an LMG is shown in Fig. 1 and more detailed descriptions can be found in [1–4]. The LMG shown in the figure is actually highly idealized, assuming lamels that are strictly vertical, with no sidewall roughness and surface contamination.

LMGs are currently fabricated using a variety of techniques, such as Reactive Ion Etching (RIE) [5, 6] and Bosch Deep Reactive Ion Etching (Bosch DRIE) [7, 8]. However, the effect of process specific features or any process artefacts of these fabrication methods may lead to non-ideal structures, such as non-rectangular shapes, materials intermixing and roughness. These may influence the reflectance of LMGs and such phenomena have not yet been investigated. Amongst the most important of such fabrication effects are the typical sidewall scalloping and surface contamination due to the passivation cycle from Bosch DRIE [7–9] and the non-rectangular and often over-etched lamel profile when using standard RIE [5, 6].

In this work, we present the first theoretical analysis that takes into account the main structural properties imposed by fabrication effects. We derive a general Coupled Waves Approach (CWA) to study the optical performance, in terms of bandwidth and peak reflectivity, of as-fabricated LMGs. This approach is well-suited for the soft x-ray spectral range and allows for the implementation of arbitrary lamellar shapes, arbitrary depth distributions of the dielectric permittivity in the multilayer structure and can be used without limitations on the grating period, lamellar width or number of bi-layers in the multilayer structure [1, 2]. Our analysis of fabricational artefacts starts with the relatively simple case of passivation layers, which were found to mainly reduce peak reflectivity due to increased absorption. Next, we examine non-rectangular lamel profiles and demonstrate that slightly positive tapered profiles can narrow the spectral reflectivity. Finally, we investigate the important case of a complex sidewall profile, specifically scalloping as caused by Bosch DRIE. Scalloping was determined to cause additional Bragg peaks. We also derive conditions for which these Bragg peaks do not significantly

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Fig. 1. Schematic cross section of a highly idealized LMG. An incident beam from the left (In), under grazing angle $\theta_0$, is reflected from the multilayer and diffracted into multiple orders (Out) under grazing angle $\Phi_j$ by the grating structure. The multilayer is built up from $N$ bi-layers (thickness $d$) consisting of an absorber ($A$) and spacer material ($S$) with thickness-ratio $\gamma$. The grating structure is defined by the period $D$ and lamel width $\Gamma D$ (i.e., $\Gamma < 1$ is the ratio of the lamel width to the grating period).

affect LMG optical performance.

2. Generalized coupled wave equations

To analyze the influence of fabricational effects on LMG reflectance, we deduce equations via the Coupled Waves Approach (CWA), which are more general as compared to those in our previous works [1, 2]. We now consider an arbitrarily shaped lamel profile as shown schematically in Fig. 2. Here, curves 1 and 2 are the sidewalls of the lamel, such that the space between these curves is filled by a ML structure. In addition, layers of thickness $h$ on the sidewalls of the lamel, indicated by curves 3 and 4, are considered. Here, we refer to these layers as being cover layers as the theory describing these layers is valid for both contamination layers as well as deliberately grown capping layers that may be applied to protect LMG structures. Curves 1 and 3 as well as curves 2 and 4 are assumed for simplicity to be equidistant, while curves 1 and 2 (as well as 3 and 4) are mirror inverted with respect to the Z-axis. Suppose the right sidewall depicted by curve 2 is described by a single-valued function $x = p(z)$. Then $x = -p(z)$ describes the shape of the opposite wall, i.e. curve 1, and $x = \mp p(z) \mp h$ can be written for curves 3 and 4, respectively. It was assumed that the lamel width and cover layer thickness are sufficiently small such that $2(p(z) + h)$ does not exceed the grating period $D$ at any $z$.

The spatial distribution of the dielectric constant is then written as:

$$
\varepsilon(x, z) = \begin{cases} 
1 & \text{if } z < 0; \\
1 - \chi(z)U(x, z) - \chi_{cov}V(x, z) & \text{if } 0 \leq z \leq H \\
1 - \chi_{sub} & \text{if } z > H
\end{cases}
$$

(1)
Fig. 2. Schematic cross section of a general shaped lamel. Curves 1 and 2 indicate the sidewalls of the ML structure and are described by the functions $\pm p(z)$. A cover layer with thickness $h$ is indicated in red by curves 3 and 4. $\Gamma_{\text{top}}$ and $\Gamma_{\text{bottom}}$ indicate the $\Gamma$-ratio at the top and bottom of the lamel, respectively.

where $\chi(z)$ is the polarizability of a multilayer structure varying with the depth, while $\chi_{\text{cov}}$ and $\chi_{\text{sub}}$ are the constant polarizability of the cover layer and substrate, respectively. The function $U(x,z) = 1$ if the point $(x,z)$ is placed inside multilayer structure and $U = 0$ otherwise. Similarly, the function $V(x,z) = 1$ if the point $(x,z)$ is placed inside the cover layer and otherwise equals zero.

Assuming the dielectric constant to be a periodic function of $x$, we represent the functions $U$ and $V$ as the Fourier series

$$U(x,z) = \sum_{n=-\infty}^{+\infty} U_n(z) \exp(2i\pi nx/D) ; \quad V(x,z) = \sum_{n=-\infty}^{+\infty} V_n(z) \exp(2i\pi nx/D) ,$$

(2)

where

$$U_n(z) = \frac{1}{\pi n} \sin \left( \frac{2\pi np(z)}{D} \right) ; \quad V_n(z) = \frac{2}{\pi n} \sin \left( \frac{\pi nh}{D} \right) \cos \left[ \pi n \left( \frac{2p(z)}{D} + \frac{h}{D} \right) \right] .$$

(3)

with $U_0(z) = 2p(z)/D$ and $V_0 = 2h/D$. We note that Eq. (3) differs from those used in our previous investigations [1, 2] as the point $x = 0$ is now chosen to be in the center instead of at the left side of the lamel. Transforming the coordinates of the previous work as $x' = x - \Gamma D/2$ yields the same coefficients as used here.

We use the Rayleigh expansion of the field:

$$E(x,z) = \sum_{n=-\infty}^{+\infty} F_n(z) \exp(iq_n x) ; \quad q_n = q_0 + \frac{2\pi n}{D} ; \quad q_0 = k \cos \Theta_0 ; \quad k = \frac{2\pi}{\lambda} .$$

(4)

Equations (2)-(4) are substituted into the wave equation $\nabla^2 E(x,z) + k^2 \varepsilon(x,z) \cdot E(x,z) = 0$. 

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From this we obtain an infinite system of coupled wave equations

\[ F_n''(z) + \kappa_n^2 F_n(z) = k^2 \sum_m [\chi(z)U_{n-m}(z) + \chi_{\text{con}}V_{n-m}(z)] F_m(z), \]  

for \( n = 0, \pm 1, \pm 2, \ldots \) with boundary conditions

\[ F_n'(0) + i\kappa_n F_n(0) = 2i\kappa_n \delta_{n,0}; \quad F_n'(L) - i\kappa_n^{(s)} F_n(L) = 0, \]

where \( \kappa_n = \sqrt{k^2 - q_n^2} \) and \( \kappa_n^{(s)} = \sqrt{k^2 - \varepsilon_{\text{sub}} - q_n^2} \) are the Z-components of the wave vector for the \( n^{th} \) diffraction order in vacuum and the substrate, respectively, and \( \delta_{n,0} \) is the Kronecker symbol.

We represent the diffracted field \( F_n(z) \) as a superposition of two waves traveling in opposite directions along the Z-axis

\[ F_n(z) = A_n(z) \exp(i\kappa_n z) + C_n(z) \exp(-i\kappa_n z), \]

and we impose an additional requirement for the unique determination of the wave amplitudes \( A_n \) and \( C_n \)

\[ \frac{dA_n(z)}{dz} \exp(i\kappa_n z) + \frac{dC_n(z)}{dz} \exp(-i\kappa_n z) = 0. \]

Substituting (7)-(8) into (5), we obtain a system of first-order differential equations

\[ \frac{dA_n(z)}{dz} = -\frac{i k^2}{2\kappa_n} \sum_m W_{n-m}(z) [A_m(z) \exp(i(\kappa_m + \kappa_n)z - i(\kappa_m - \kappa_n)z)] \]

\[ \frac{dC_n(z)}{dz} = +\frac{i k^2}{2\kappa_n} \sum_m W_{n-m}(z) [\chi(z)U_{n-m}(z) + \chi_{\text{con}}V_{n-m}(z)], \]

where

\[ W_{n-m}(z) = \chi(z)U_{n-m}(z) + \chi_{\text{con}}V_{n-m}(z), \]

and with boundary conditions

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

where the dielectric constant of the substrate is set to unit.

We are mainly interested in the specular reflection of LMGs operating in the single-order regime. Such operation is achieved when the grating period \( D \) and lamel-to-period ratio \( \Gamma \) are reduced to fulfill:

\[ \Gamma D \cdot \Delta \Theta_{\text{MM}} << d, \]

where \( d \) is the bi-layer thickness and where \( \Delta \Theta_{\text{MM}} \) is the acceptance angle for Bragg reflection by the conventional ML mirror (without a grating structure). The first and higher diffraction orders then fall out of the acceptance angle and the incident beam is only reflected in a single diffraction order. It was derived in [1] that the reflectivity of a single-order LMG is the same as that of a conventional ML mirror with the material polarizability reduced by a factor \( \Gamma \). In the limit of an ideal, semi-infinite and strictly periodic ML stack, single-order operation reduces the spectral bandwidth by a factor of \( 1/\Gamma \) while the peak reflectivity remains as high as that of a conventional ML mirror [1, 2].
In the single-order LMG regime, we can neglect the interaction of the incident beam with higher diffraction orders and keep only equations of system (5) with \( n = 0 \) [1]. The equation describing the interaction of the field with a single-order LMG is then given by

\[
F_0''(z) + k^2 \left( \sin^2(\Theta_0) - \chi_{\text{eff}}(z) \right) \cdot F_0(z) = 0, \tag{14}
\]

which is simply the wave equation for radiation propagating inside a 1D layered medium, whose polarizability varies in the depth as

\[
\chi_{\text{eff}}(z) = \chi(z) \cdot 2p(z)/D + \chi_{\text{cov}} \cdot 2h/D. \tag{15}
\]

Equations (9)-(15) enable us to analyze for the first time the optical effect of various LMG structures as obtained from fabrication, without the limitation to an idealized structure. Equations (14)-(15) are well suited for preliminary physical analysis, while the CWA equations (9)-(10) are used for the numerical calculations.

In this analysis, we simulated the same single-order LMG as used in [1, 2]. The parameters of the idealized LMG are \( D = 300 \text{ nm}, \Gamma = 0.3, N = 150, d = 6 \text{ nm} \) and \( \gamma = 0.33 \). The values of the complex polarizability used at the photon energy of the incident radiation of 183.4 eV are \( \chi(Mo) = 2.61 \cdot 10^{-2} - i5.77 \cdot 10^{-3} \) and \( \chi(B_4C) = 4.43 \cdot 10^{-5} - i1.08 \cdot 10^{-5} \) [10, 11]. For the numerical calculations, 5 diffraction orders are taken into account. The \( 0^{th} \) order efficiency is referred to as the reflectivity.

3. Cover layers

We begin our analysis by examining the effect of a cover layer. As previously stated, this layer can be the result of contamination or can be deliberately grown as a capping layer to protect the ML structure. For this analysis, we first briefly recall the simplest case of an LMG with a rectangular lamel profile \( (p(z) = \Gamma D/2) \) and no cover layer \( (h = 0) \) as previously investigated in detail in [1, 2, 12]. In this case, the effective polarizability \( \chi_{\text{eff}}(z) = \Gamma \chi(z) \) corresponds to a conventional ML mirror with material densities reduced by a factor of \( \Gamma \). The maximal achievable peak reflectivity of an LMG is then the same as that of a conventional ML mirror, while the penetration depth of the SXR wave is increased by a factor of \( 1/\Gamma \). As a result, the reflectivity bandwidth is spectrally narrowed by the factor \( \Gamma \). In other words, single-order LMGs allows to obtain any desired resolution while maintaining high peak reflectivity under the assumption that the ML structure contains sufficient bi-layers.

In the case of a cover layer, with thickness \( h \) and polarizability \( \chi_{\text{cov}} \), on the lamel sidewalls, the effective polarizability of each layer in the ML stack is increased by the same value such that \( \chi_{\text{eff}}(z) = \Gamma \chi(z) + 2h/D \cdot \chi_{\text{cov}} \). The penetration depth of the SXR wave into the ML structure is mainly determined by the contrast in polarizability of the materials (absorber and spacer) in the ML structure \( \text{Re}(\chi_A - \chi_S) \) rather than by absorption if \( \text{Re}(\chi_A - \chi_S) \gg \text{Im}(\chi_A) \) [13]. This condition is indeed fulfilled for the Mo/B_4C structure \( \text{Re}(\chi_A - \chi_S) \approx 4 \cdot \text{Im}(\chi_A) \) analyzed in the present paper. Evidently, the presence of a cover layer does not change the polarizability contrast and, hence, only weakly affects the penetration depth of the SXR wave. As a result, the reflectivity bandwidth of an LMG is also only minimally affected.

The cover layer also increases the absorption of SXR radiation by the LMG which, due to energy conservation, decreases the peak reflectivity. To investigate this effect in more detail, we study the effect of the cover layer on the effective polarizability of each layer in the ML stack. As a high-Z material is typically used as absorber, meaning \( \text{Im}(\chi_A) \gg \text{Im}(\chi_{\text{cov}}) \), the cover layer can be concluded to have a very limited effect on the absorption of those layers. However, a low-Z material with a minimal absorption coefficient for the incident radiation is usually used as a spacer. This means that \( \text{Im}(\chi_S) < \text{Im}(\chi_{\text{cov}}) \). Taking into account that the field intensity...
maxima are placed just inside the spacer layers [15], we can conclude that the cover layer may significantly increase the absorption by the spacer layers and, hence, result in decreased LMG reflectivity. A criteria for which a minimal effect on peak reflectivity is observed can be derived by ensuring that the contribution of the cover layer absorption \( h/D \cdot \Im(\chi_{cov}) \) to the spacer layer absorption \( \Gamma \Im(\chi_S) \) would be negligibly small. This requires that the cover layer is sufficiently thin, expressed as:

\[
h << \frac{\Gamma D}{2} \frac{\Im(\chi_S)}{\Im(\chi_{cov})}
\]

The effect of a cover layer on the optical performance of an LMG is demonstrated by Fig. 3, where the 0\(^{th}\) and ±1\(^{st}\) diffraction orders are depicted for various cover layer thicknesses. Here, we assume a Bosch process would result in the deposition of a light material (\( C_nF_{2n} \)) passivation layer. According to Eq. (16), layer thicknesses below 20 nm should have a negligible effect on the LMG optical performance. It can be seen in Fig. 3 that the effect on the 0\(^{th}\) and ±1\(^{st}\) orders is indeed very small for such thicknesses as demonstrated by the calculations with \( h = 4 \text{ nm} \). For this layer thickness, the peak reflectivity is only reduced by 2 % and the angular position and bandwidth are not significantly affected as compared to an uncovered LMG. However, at a layer thickness of 20 nm the effect of the cover layer becomes apparent. The peak reflectivity is decreased significantly from 38 to 28 % and the peak is shifted as compared to the uncovered LMG. The FWHM spectral bandwidth corresponding to the FWHM angular width in Fig. 3 increased only very slightly from 1.468 to 1.475 eV, i.e. less then 1 %, due to the 20 nm cover layer. The figure clearly demonstrates that the bandwidth is only negligibly affected by the cover layer, whereas the peak reflectivity can be significantly reduced for layer thickness.

Fig. 3. Calculations of the diffraction efficiencies of the 0\(^{th}\) (reflectivity) and ±1\(^{st}\) orders for various thicknesses of a \( C_nF_{2n} \) cover layer on a Mo/B\(_4\)C LMG at the incident SXR energy E of 183.4 eV. The cover layers result in a negligible increase in bandwidth, but can strongly reduce the peak reflectivity and result in a shift of peak position for thicker layers. The parameters of the LMG are \( D = 300 \text{ nm}, \Gamma = 0.3, N = 150, d = 6 \text{ nm} \) and \( \gamma = 0.33 \). The values of the complex polarizability used are \( \chi(Mo) = 2.61 \cdot 10^{-2} - i5.77 \cdot 10^{-3} \) and \( \chi(B_4C) = 4.43 \cdot 10^{-3} - i1.08 \cdot 10^{-3} \).
The cover layer clearly also results in a shift of the peak position for layer thicknesses that do not fulfill Eq. (16). This shift is caused by the change in optical path length due to the cover layer, comparable to the shift in peak position due to the $\Gamma$-ratio for single-order LMGs as discussed in [2]. A general statement on the maximum acceptable cover layer thickness cannot be given as this will depend on the cover layer material and working wavelength, but in general its thickness should not exceed several nanometers.

4. Non-rectangular lamell profile

A frequently occurring fabrication artefact of LMGs is a tapering of the lamellar profile. To analyze the effect of such a tapered profile, we assume the sidewall profile is described by the trapezoidal function $p(z) = D\Gamma_{\text{top}}/2 + D(\Gamma_{\text{bottom}} - \Gamma_{\text{top}})z/(2H)$ for definiteness. The taper of the profile is then given by $\tan^{-1}(D/(2H) \cdot |\Gamma_{\text{bottom}} - \Gamma_{\text{top}}|)$. A positive taper thus indicates that $\Gamma_{\text{top}} < \Gamma_{\text{bottom}}$ and a negative taper that $\Gamma_{\text{top}} > \Gamma_{\text{bottom}}$. The effect of various tapers on the LMG reflection were calculated assuming the LMG as described previously and keeping the average $\Gamma$ of the lamell constant at 0.3.

Results of these calculations are shown in Fig. 4. It can be seen that the effect of taper can be quite significant. We note that the simulated negative taper of $-5^\circ$ is quite unrealistic as this corresponds to a lamell width of only 10 nm at the bottom of the structure as compared to 170 nm at the top. This negative taper resulted in an increase of the $0^{th}$ order bandwidth of 25%. However, the peak reflectivity was not significantly affected. For a positive taper of the same absolute value, i.e. $+5^\circ$, the bandwidth remained constant and the peak reflectivity was practically the same. However, at lower positive ($\approx 2-3^\circ$) tapers the bandwidth was actually slightly narrower (from 1.47 down to 1.40 eV) than for the rectangular profile. Furthermore, the positive taper showed increased background suppression at angles just outside the main Bragg peak.

![Fig. 4. Calculated $0^{th}$ and $\pm1^{st}$ diffraction order efficiencies for rectangular as well as positively and negatively tapered lamell profiles with the same average $\Gamma$-ratio of 0.3 at the incident energy of 183.4 eV. The LMG parameters are the same as for Fig. 3.](image)

The difference in effects of a positive and negative taper can be explained by considering...
the effect of the taper as a monotone change in effective density in the depth of the ML stack. For a positive taper the density is reduced near the top of the structure, which may result in a deeper penetration of waves into the LMG and thereby resulting in a bandwidth reduction. On the other hand, a negative taper results in increased effective density near the top of the structure and actually limits the penetration depth of the wave into the LMG resulting in increased bandwidths.

5. Scalloping

A second example of a frequently occurring fabricational artifact consists of sidewall scalloping. This sidewall scalloping, of which an example can be seen in Fig. 5(a), is inherent to the working principle of Bosch Deep Reactive Ion Etching (DRIE) fabrication process. In Bosch DRIE, etching and passivation cycles are performed in a sequential manner to obtain a directional pattern transfer and a high aspect-ratio of the lamels. The etching itself is performed semi-isotropically in both the vertical and lateral direction. After the etching cycle, a passivation layer is deposited to prevent further etching. This passivation layer is removed in the vertical direction by physical etching during the next etch cycle. During this cycle, semi-isotropic etching is continued where the passivation layer is removed. The sequential nature of this process results in a typical scalloped sidewall profile. We suppose, for definiteness in modeling, that the sidewall scalloping can approximately be described by a periodic function

$$p(z) = \Gamma D/2 + a/2 \cdot \sin(2\pi z/l)$$

where $a$ is the scallop amplitude, $l$ is the scallop length and $\Gamma D$ is the average lamel width as depicted in Fig. 5(b).

For a preliminary physical analysis of the effect of scalloping we investigate the description of the effective polarizability $\chi_{eff}(z) = \chi(z) \cdot 2p(z)/D$, which is then given by the product of two periodic functions with periods $d$ and $l$. If the ratio $d/l$ is an irrational number, the function $\chi_{eff}(z)$ is not periodic. Expanding the functions $\chi(z)$ and $p(z)$ into the Fourier series, we find that $\chi_{eff}(z)$ contains terms with four main periods $d_j (j = 0 - 3)$, namely $d_0 = d$; $d_1 = l$; $d_2 = d/(1 + d/l)$ and $d_3 = d/(1 - d/l)$ as well as higher harmonics with periods $d_j/n (n = 2, 3, ...).$ Though not used here, we note a similar layered structure containing terms with different periods was analyzed in detail in [14] by Balakireva et al. to model the problem.
of simultaneous reflection of two arbitrary wavelengths from a multilayer mirror.

As in [1, 2], we are interested in the first order Bragg reflection and we therefore neglect the higher order terms in the Fourier series. The depth-distribution of the effective polarizability is then written in the simplified form:

\[
\chi_{\text{eff}}(z) \approx \Gamma \zeta + \frac{a}{D} \chi \left( \frac{2 \pi z}{d_1} \right) + (\chi_\Lambda - \chi_0) \frac{\sin(\pi \gamma)}{\pi}.
\]

\[
2 \Gamma \cos \left( \frac{2 \pi z}{d_0} - \pi \gamma \right) + \frac{a}{D} \sin \left( \frac{2 \pi z}{d_2} - \pi \gamma \right) - \frac{a}{D} \sin \left( \frac{2 \pi z}{d_3} - \pi \gamma \right)
\]

If the grazing angle of the incident beam is varied, resonant Bragg reflection can possibly be observed from each of the terms in Eq. (17). However, because the scallop period \( l = d_1 \) is typically much larger than the ML mirror period \( d_0 \), Bragg reflection from this term occurs at very small grazing angles and is therefore not considered below. The terms with periods \( d_2 \) and \( d_3 \) may be close to the ML mirror period \( d_0 \) if the scallop length \( l \) is large enough. As a result, specular reflection is now expected to occur at three different Bragg angles such that \( \lambda = 2 d_j \sin(\Theta_{m=0}^{(j)}) \), where \( m = 0 \) indicates the \( j^\text{th} \) diffraction order and \( j = 0, 2, 3 \) is the index of the period. Similarly, three diffraction peaks are also expected for any \( n \)\( \text{th} \) order such that \( \lambda = 2 d_j \left( \sin(\Theta_{m}^{(j)}) + \sin(\Phi_{m}^{(j)}) \right) \), where the diffraction angle \( \Phi_{m}^{(j)} \), i.e. the grazing angle of the outgoing diffracted beam, is determined by the grazing incidence angle via the grating equation \( m \lambda = D \left( \cos(\Theta_{m}^{(j)}) - \cos(\Phi_{m}^{(j)}) \right) \). The angle \( \Phi_{m}^{(j)} \) can be referred to as the quasi-Bragg resonance angle and is comparable to the blaze angle in the theory of conventional diffraction gratings. From Eq. (17), we determined that period scalloping can therefore be considered to be equivalent to the appearance of a number of embedded diffraction gratings with the same \( D \) and \( \Gamma \), but with different ML periods \( d_j \). As the scallop amplitude \( a \) is typically \( << 2 \Gamma D \), as can be seen in Fig. 5(a), the amplitude of the scallop-induced Bragg side peaks corresponding to the periods with index \( j = 2 \) and \( 3 \) is small and we can expect that their effect on the main reflectivity peak is negligible.

This is demonstrated by Fig. 6, where the specular reflection and \( \pm 1 \)\( \text{st} \) order diffraction peaks were calculated using eqs. (9)-(10). Here, the dashed curves show the calculated peaks from an LMG without scalloping and, for comparison, the solid curves show the same angular (and equivalently energetic) range for an LMG with scalloped sidewalls with a scallop length of 150 nm. For the scallop amplitude, which is typically only in the order of 5-10 nm, we took an increased value of 80 nm for better visibility and illustration of the scallop-induced Bragg side peaks. According to Eq. (17), the scallop-induced side peaks should arise on the reflectivity curve corresponding to Bragg reflection from the periods \( d_2 \) and \( d_3 \). These side peaks are indicated by red arrows in Fig. 6. In spite of the very large scallop amplitude, neither the height nor the bandwidth of the main peak is found to be affected by the scallops. Similar scallop harmonics also arise next to the \( \pm 1 \)\( \text{st} \) order diffraction peaks and, in contrast to the specular reflection peak, the efficiency of these orders decreases noticeably due to scalloping. The bandwidth of the higher diffraction orders was also reduced by almost 10% when increasing the scallop width from 0 to 80 nm.

The appearance of such scallop harmonics raises the question to what extent scalloping in LMGs is acceptable for practical applications such as SXR spectroscopy. Our calculations show that the amplitude of the scallop-induced peaks can be significantly reduced by decreasing the scallop amplitude to below 10 nm. This is demonstrated by the dotted curves in Fig. 6, which are in good agreement with the dashed curves calculated in the absence of scalloping as these curves differ by \( < 1 \% \) in peak reflectivity.

Although the coupling of waves reflected and diffracted from the different embedded gratings
Fig. 6. $0^{th}$ and $\pm 1^{st}$ order efficiencies for various scallop widths $a$ at a scallop length $l$ of 150 nm at the incident energy of 183.4 eV. The additional scallop harmonics of the specular reflection are indicated by red arrows. The LMG parameters are the same as for Fig. 3.

is typically very weak, as we have shown in the previous example, there exists a specific case when this coupling may be strong. This occurs when the Bragg angle of reflection from the ML with period $d_0$ coincides with the quasi-Bragg angle of diffraction from the gratings with ML period $d_2$ or $d_3$, i.e. when $\Theta_0^{(0)} = \Theta_2^{(2)}$ or $\Theta_0^{(0)} = \Theta_3^{(3)}$. In these cases the incident wave effectively excites at least two waves, namely the specularly reflected wave from the main grating with period $d_0$ and the scallop-induced peak from a higher grating order. As at least two waves can be excited, the LMG is actually no longer in single-order operation even for LMGs that do fulfill the single-order condition (13). This results in a loss of peak reflectivity as the incident energy is then distributed over both the specularly reflected and diffracted waves.

To determine the conditions for this effect to occur, simultaneous resonant excitation of the specularly reflected and, for definiteness, $+1^{st}$ order diffracted waves (i.e. the case when $\Theta_0^{(0)} = \Theta_2^{(2)}$) are examined here. This yields the following system of equations:

\[
\begin{align*}
\lambda &= 2d_0 \sin(\Theta_0^{(0)}) \\
\lambda &= d_2 \left( \sin(\Theta_0^{(0)}) + \sin(\Phi_{+1}^{(2)}) \right) \\
\lambda &= D \left( \cos(\Theta_0^{(0)}) - \cos(\Phi_{+1}^{(2)}) \right). 
\end{align*}
\]  

Taking into account that $\lambda \ll D$, i.e. $\Phi_{+1}^{(2)}$ is close to $\Theta_0^{(0)}$, and expanding $\sin(\Phi_{+1}^{(2)})$ and $\cos(\Phi_{+1}^{(2)})$ in a series near $\Theta_0^{(0)}$, we find that the Eqs. (18) are fulfilled if the scallop length obeys the condition

\[
l_w \approx D \tan(\Theta_0^{(0)}),
\]

where $l_w$ indicates the worst scallop length, i.e. the scallop length for which the $0^{th}$ order peak reflectivity is most strongly affected by the scallop harmonics. The same derivation can also be
performed for quasi-Bragg resonance arising from period $d_3$, which gives the same result.

The above case is demonstrated in Fig. 7 where the specular reflectivity as well as $\pm 1^{st}$ orders diffraction efficiencies are shown for the worst scallop length of 205 nm, as derived from condition (19), at various scallop amplitudes. It can easily be seen that for the scallop amplitude of 80 nm (solid curve) the scallop-induced peaks from the diffraction orders, as indicated by the red arrows, strongly overlap the main Bragg peak of the specularly reflected wave. As a result, the peak reflectivity drops sharply as compared to the case with no scalloping (dashed curves). A similar effect is also observed for $\pm 1^{st}$ order diffraction peaks. As for the scallop length of 150 nm, decreasing the scallop amplitude down to 10 nm (dotted curves) results in a significant reduction of the scallop harmonic amplitude and is very similar ($< 1\%$ difference in peak efficiencies) to the case without scalloping.

Please note that existing technologies allow for the fabrication of LMGs with scallop widths below 10 nm [7, 8]. Furthermore, negative effects of scalloping could also be possibly reduced by adapting fabrication technologies to result in aperiodic scalloping.

6. Conclusions

We have derived generalized equations for our Coupled Waves Approach (CWA) to determine the effect of various fabricational features on the optical performance, in terms of bandwidth and peak reflectivity, of Lamellar Multilayer Gratings (LMG). Using these generalized equations, we first analyzed the effect of cover layers on the sidewalls of the lamels. Such layers primarily reduce peak reflectivity due to increased absorption, but also have a small effect on bandwidth. Criteria for layer thicknesses that have negligible effects on the LMG optical performance were derived.

The effect of realistic lamel profiles was investigated next. In particular negative tapers, i.e.

![Graph showing specular reflectivity and diffraction efficiencies for various scallop lengths and amplitudes. The graph includes curves for $l=205\,\text{nm, } a=0\,\text{nm}$, $l=205\,\text{nm, } a=10\,\text{nm}$, and $l=205\,\text{nm, } a=80\,\text{nm}$, with $\pm 1^{st}$ order efficiencies at the grazing angle.]
when the lamel is wider at the top than at the bottom, were determined to have a strong effect on the optical performance of the LMG. This is because a negative taper can be seen to result in increased density near the top of the structure, thereby limiting the contribution of reflections from lower bi-layers to the interference and thus resulting in increased bandwidths. For positive tapers, the bandwidth can actually be reduced as reflections from lower bi-layers then contribute more to the interference. For the same average Γ-ratio, the peak reflectivity does not significantly differ between idealized, rectangular structures and those with positive or negative tapers.

Finally, the effect of scalloping on the LMG optical performance was determined. We derived that for specific scallop lengths the incident wave can excite both the specularly reflected wave as well as a scallop-induced side peak from a different grating order. This results in a loss of peak efficiency as not all incident energy is diffracted into a single order, i.e. the LMG is no longer in single-order operation even for LMGs that do fulfill the single-order condition. We found that such loss in reflectivity can be avoided by ensuring the scallop length obeys a certain condition or that the scallop amplitude is kept small, typically below 10 nm. If one of these criteria for the scallop dimensions is obeyed, which is technologically feasible, the coupling between the incident and scallop harmonic wave is then small and the optical effect is therefore also small.

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