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Breaking the efficiency limit for high-frequency blazed multilayer soft x-ray gratings: Conical vs classical diffraction

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High-frequency multilayer-coated blazed diffraction gratings (HFMBGs) are most promising elements for ultrahigh resolution soft x-ray spectroscopy. As it has been demonstrated recently [Voronov *et al.*, Opt. Express **23**, 4771 (2015)], the efficiency limit for in-plane diffraction can exceed 2–3 times, in higher orders too, when the period of a HFMBG is shorter than an attenuation length for soft x-rays and a bilayer asymmetry is designed. In this letter, using numerical experiments based on the rigorous electromagnetic theory, a possibility of off-plane diffraction and symmetrical multilayer coatings to enhance the efficiency of soft-x-ray high-order HFMBGs very closely to the absolute limit, i.e., 0.92–0.98 of the reflectance of the respective W/B4C multilayer, has been demonstrated. *Published by AIP Publishing.* [http://dx.doi.org/10.1063/1.4962395]

High-frequency multilayer-coated gratings are most promising diffraction elements for many x-ray applications in astrophysics, plasma diagnostics, lithography, beam splitting, etc. A grand challenge in hard and soft x-ray spectroscopy is to enhance, at a high level of throughput, the resolving power of monochromators/spectrometers from 10^4 up to 10^6. This need is driven mainly by the revolution requirements of Resonant Inelastic X-ray Scattering (RIXS).[1] Using high-frequency gratings in off-plane (conical diffraction) mounts leads to compact pattern geometry, high efficiency, high dispersion, and high spectral resolution compared to respective low- and mid-frequency gratings working in in-plane (classical) mounts.[2] The grating structure in the grazing-incidence off-plane configuration can be also a rather efficient amplitude beam splitter for hard x-rays, e.g., in the coherent beam from a free electron laser.[3] Off-plane reflection gratings offer an effective way to reach simultaneously the high resolution and throughput required by the next generation of soft x-ray observatories.[4,5] Such gratings may also be blazed and/or multilayer to diffract a great amount of the total reflected energy to a principal (blazed) order and to increase a grazing incidence angle, thus, reducing significantly a noise-to-signal ratio and the required detecting area. In recent years, soft-x-ray and extreme UV (EUV) high-frequency (with a period of 50–200 nm) multilayer blazed gratings (HFMBGs) with high spectral resolution and high efficiency have been fabricated by different techniques.[6–10] The efficiency of soft x-ray HFMBGs depends significantly on the parameters of the triangular substrate and the multilayer. HFMBGs have the superior performance as compared to similar low- and mid-frequency gratings, which are traditionally used in soft x-ray instrumentation. The dense multilayer periods become semi-transparent in soft-x-rays, and they reduce the shadowing effect which causes efficiency loss and results in efficiency gain as compared to the efficiency of low-frequency gratings. It has recently been demonstrated, using numerical and synchrotron radiation experiments,[11–13] that the efficiency limit (the Maystre-Petit factor) for classical diffraction can exceed 2–2.5 times, in higher orders too, when the period of a multilayer blazed grating is shorter than an attenuation length for soft x-rays and a bilayer asymmetry is designed. However, one needs to understand how to optimize the performance of the HFMBG by an optimum choice of the mount, grating substrate, and multilayer parameters, as well as take into account physical and fabrication limitations. In this letter, using exact numerical experiments on the basis of the rigorous electromagnetic theory—an equivalent of accurate synchrotron radiation measurements,[2,4,7,11–15] we demonstrate a possibility of conical diffraction using mid blaze angles and coatings without a bilayer asymmetry to enhance the efficiency of soft-x-ray HFMBGs closely to the absolute limit, i.e., the reflectance of the respective multilayers.

We consider a HFMBG with the period $d = kd_{\min}$, where k is an integer. If gratings have the same blaze angle ζ and the same multilayer coating with the bilayer spacing Δ, the blaze condition for the kmth diffraction order, m is an integer, of a HFMBG should satisfy both the Grating equation and the Bragg condition

$$m\Delta = d_{\min} \sin \zeta. \qquad (1)$$

The angles of incidence and diffraction are the same for such gratings. At a fixed parameter $m\Delta$, a high value of $d_{\min}$ requires a small value of ζ that is difficult to produce with a high quality (the range of low-frequency first-order grazing-incidence gratings). And vice versa, a small value of $d_{\min}$ requires a large value of ζ that is also difficult to fabricate (the range of echelles). In accordance with (1), the minimal depth of the grating should be higher than one bilayer spacing so that for $m\Delta/d \tilde{<} 1$, ζ approaches to 90°. Evidently, an optimum is in mid-range values of ζ from a few degrees up to about 10° that is a range for bulk mid-frequency gratings working currently in many in-plane diffraction spectral instruments. The main disadvantage of such gratings is low

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diffraction efficiencies η due to shadowing. The influence of shadowing is also one of the main questions arising under switching to analysis of HFMBGs with mid values of ζ working both in in-plane and off-plane mounts. According to the Maystre-Petit formula which is valid for both classical and conical diffractions[16] the gratings should have the same maximal diffraction efficiency η_{MP} for the kmth blazed order

$$\eta_{MP} = R \min[\cos\alpha/\cos\beta_{km}, \quad \cos\beta_{km}/\cos\alpha], \qquad (2)$$

where R is a reflectance of a blazed facet surface, and α and β_{km} are incidence and diffraction polar (in-plane) angles, respectively, measured from the normal to the grating plane. In in-plane mountings, the performance of blazed gratings is affected by shadowing effects and η of a blazed order reduces in accordance with the Maystre-Petit geometrical factor of asymmetry of diffraction. However, our simulations and measurements reveal a pronounced effect of the groove density on η of MBGs. The recent and earlier investigations[11,17] show that η of blazed orders of in-plane HFMBGs can be higher than predicted (2) by a significant factor of about 2–3. For grazing-incidence off-plane diffraction, the Maystre-Petit factor can be easily set to one and the efficiency predicted by (2) should be equal to the reflectance of a grating coating; however, it has never been studied for HFMBGs.

The dependence of the diffraction efficiency on the groove density of HFMBGs working in the in-plane configuration is shown in Fig. 1 for a wide range of periods $d = 28.6 \div 2000$ nm with high space resolution and high accuracy for the TE polarization (the electric field vector is perpendicular to the incidence plane and parallel to grooves) of the incidence radiation at a wavelength $\lambda = 1.3$ nm. Note that in the soft x-ray region, polarization effects are not very strong for bulk materials at grazing incidence. However, the reflectance of multilayers in this range is more sensitive, with the difference between two principal polarizations up to a few dozen percent. All the gratings have the blaze angle $\zeta = 6°$ and the optimal W/B4C multilayer coating with

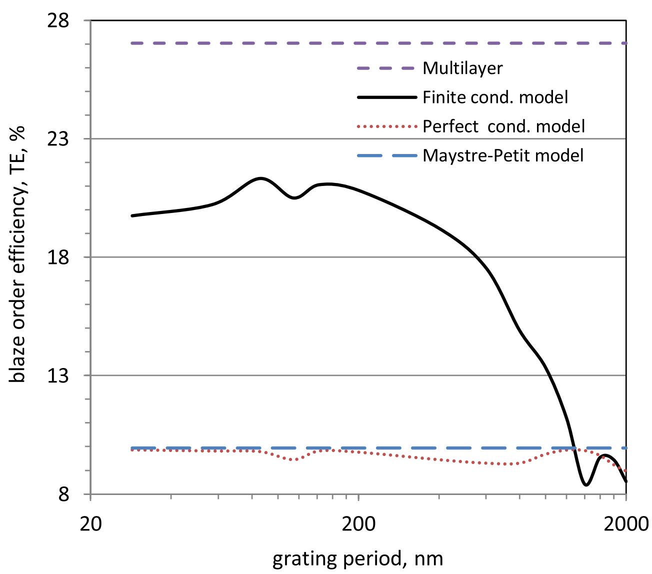

FIG. 1. Dependence of the in-plane TE-efficiency of a blazed grating coated by 40 symmetrical W/B4C bilayers vs grating period.

40 bilayers with $\Delta = 2.99$ nm and the Γ-ratio (a W layer thickness to a bilayer Δ-spacing) of 0.5 (i.e., symmetrical). The grating periods were chosen according to Eq. (1) to provide the blaze condition for a defined diffraction order. For example, the 28.6-nm-period grating has the -1st order under the blaze condition, while the 200-nm grating is optimized for the -7th blazed order. The identical geometry of in-plane diffraction allows investigation of solely the impact of the groove density on the MBG efficiency. The rigorous finite conductivity model based on the boundary integral equation method[14,15] and exact values of refractive indices[18] demonstrates in Fig. 1 that soft x-ray blazed gratings can deliver high efficiency in a high diffraction order. Low-frequency MBGs with a period of $\sim$1.2 μm and higher have $\eta \sim 10\%$ in the respective very high blazed orders that is consistent with the rigorous perfect conductivity model[14] and (2), i.e., it is determined by the multilayer reflectance and shadowing effects. For the case shown in Fig. 1, the multilayer reflectance is $\sim$27% and the geometry factor is cos 83.25°/cos 71.36° = 0.368, so η_{MP} is less than 10% for all the gratings. An increase in the groove density of a MBG results in a large efficiency gain, in opposite to decreasing η of bulk gratings with higher frequencies.[13,17] HFMBGs with $d \sim 1$ μm and less have higher efficiencies in the respective high diffraction orders. The efficiency having minor oscillations increases, on average, and eventually exceeds the scalar theory prediction more than a factor of two for gratings with $d \sim 300$ nm or less. So, the period of 300 nm can be considered in this publication as an imagined boundary between mid- and high-frequency gratings. Such high-frequency bulk reflection gratings are not practical in soft x-rays due to the efficiency limitations. Bulk gratings operate at very oblique incidence due to a critical angle limitation for total external reflection from a facet surface. In classical diffraction, this limits ζ to small values, and hence provides blazed conditions for the 1st diffraction order only. HFMBGs can operate at much larger ζ, which is much easy to produce, due to its multilayer coating, and hence can direct energy into a high diffraction order with high efficiency. Moreover, the non-grazing incidence geometry of a HFMBG mitigates shadowing effects as compared to a grazing incidence blazed bulk grating having the same groove profile. As soon as the grating period becomes shorter than the attenuation length of the radiation in the multilayer, the transparency of the grooves increases and shadowing effects are minimized, resulting in a remarkable increase in the diffraction efficiency. The efficiency of blazed gratings saturates at a smaller number of bilayers than the reflectance of plane multilayers.[11] Smaller numbers of bilayers are preferable because a multilayer tends to smooth out the triangular grooves and the smoothing increases with the coating thickness.[19] Despite the full electromagnetic optimization, the maximal ratio of the -3rd order efficiency to the respective multilayer reflectance for the grating in Fig. 1 with $d = 85.7$ nm is reached $\sim$0.79.

The off-plane grating periods were chosen according to Eq. (1) to provide the blaze condition for a defined diffraction order. The incidence polar angles for such gratings have been chosen according to

$$\alpha = -\beta = 90° - \zeta. \qquad (3)$$

Using (3), the Grating equation for conical diffraction

$$\cos\,\alpha + \cos\,\beta_{km} = km\,\lambda/(d\cos\,\varphi), \tag{4}$$

where φ is an azimuthal angle measured from the grating dispersive plane, reads

$$\lambda_{\mathrm{B}} = 2\,d\cos\,\varphi\,\sin\,\zeta/(km). \tag{5}$$

The blaze of HFMBGs is most effective for the in-plane Littrow geometry ($\varphi=0$) where incident and diffracted beams are almost normal to the surface of blaze facets (echelles). For off-plane gratings, this geometry is based on the Invariance theorem resulting in high efficiencies for short wavelengths and high azimuthal angles.[16] This theorem is proved for perfectly conducting gratings whose η can be reached 100% for one polarization state that means, taking into account finite conductivity of materials, the absolute efficiency is equal to the blaze facet reflectance (see Eq. (2)). However, this model is valid for low-frequency bulk and multilayer gratings and for one polarization only.[4,17]

The azimuthal angular dependence of the HFMBG off-plane efficiency on the groove density is shown in Fig. 2 for a wide range of periods $d=28.6\div400$ nm and different blaze angles $\zeta=3.24°$, 6°, and 12° for the TM polarization of incident radiation at $\lambda=1.3$ nm. A polar angle for gratings in this mount was chosen in accordance with (3). For gratings in the grazing-incidence off-plane mount, we refer to linearly polarized incident light whose electric field vector lies in the plane of incidence as the TE polarization (p), and define the TM polarization (s) as when the electric field vector lies almost parallel to the plane of the grating.[4] Thus, all the HFMBGs are coated with the identical W/B4C multilayer but optimized for different blazed orders. Under these conditions, η of HFMBGs under a simple scalar model (2) would be the same for all the gratings and equal to the reflectance of the multilayer ($d=\infty$ and $\zeta=0$). Indeed, the data in Fig. 2 demonstrate that off-plane soft x-ray HFMBGs can deliver even higher efficiency in a high diffraction order compared to those used in classical diffraction. For example, the grating with $d=114.3$ nm and $\zeta=6°$ has $\eta_s\sim23.7\%$ in the -4th order, and the grating with $d=105.8$ nm and $\zeta=3.24°$ demonstrates the s-efficiency higher than 25.5% in the -2nd order. The maximal ratio of $\sim$0.983 of the absolute s-efficiency to the respective multilayer reflectance is reached for the grating with $d=52.9$ nm. Even for a mid-frequency grating with $d=400$ nm and $\zeta=6°$, $\eta_s\sim20\%$.

The soft-x-ray spectral dependence of the diffraction efficiency of HFMBGs with $d=114.3$ nm and $\zeta=6°$ (-4th blaze order) and $d=200$ nm and $\zeta=7.72°$ (-9th blaze order) coated by 50 W/B4C bilayers with $\Delta=2.99$ nm and $\Gamma=0.5$ is shown in Fig. 3 for s and p polarizations of the incident radiation. The W/B4C 50-bilayer reflectance is shown in Fig. 3 for a comparison. The most inefficient is a grating working in the in-plane mount in the -9th order with $\alpha=84.97°$. It has the s-efficiency of $\sim$0.58 of the reflectance only. Another grating working in the in-plane mount in the -4th order with $\alpha=83.25°$ has $\eta_s\sim21\%$ in maxima that is $\sim$0.74 of the Bragg reflectance. The grating working in the -9th order off-plane mount with $\alpha=7.72°$ and $\varphi=77.13°$ has $\eta_s\sim23\%$ at $\lambda=1.3$ nm that is more than 37% higher than the best in-plane efficiency of the same grating. The grating with the symmetrical coating working in the off-plane mount in the -4th order with $\alpha=6°$ and $\varphi=77.24°$ has very high η in both polarizations close to the reflectance of the multilayer with the factor of $\sim$0.92. The off-plane maximum efficiencies of this grating are $\sim$24% higher in comparison with the respective in-plane efficiencies of the same HFMBG. Note that the absolute accuracy of all efficiency calculations is 0.1%.

The simulation results shown in Figs. 1–3 reveal a prominent trend which is enhanced with higher grating frequencies: increasing of η. Besides, with higher grating periods, the efficiency curves are shifted, basically towards higher incidence angles (shorter wavelengths), as compared to the reflectance curve of the multilayer. However, this trend depends also on the blaze angle and order number in

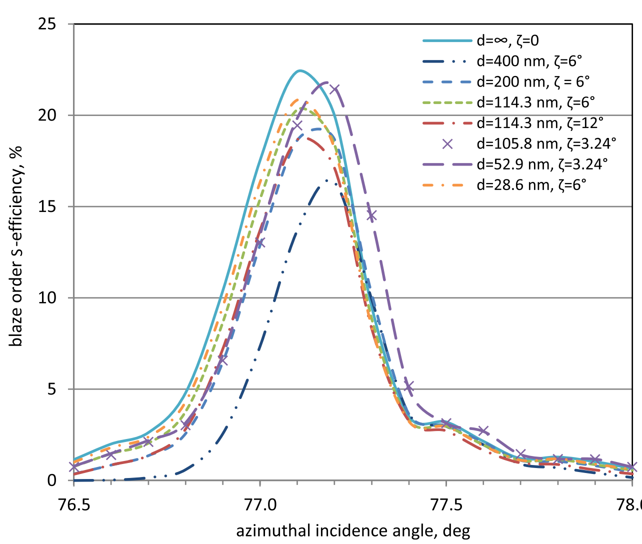

FIG. 2. Dependence of the off-plane s-efficiency of a blazed grating with the period d and the blaze angle ζ coated by 40 W/B_4C symmetrical bilayers for $\lambda=1.3$ nm vs azimuthal incidence angle.

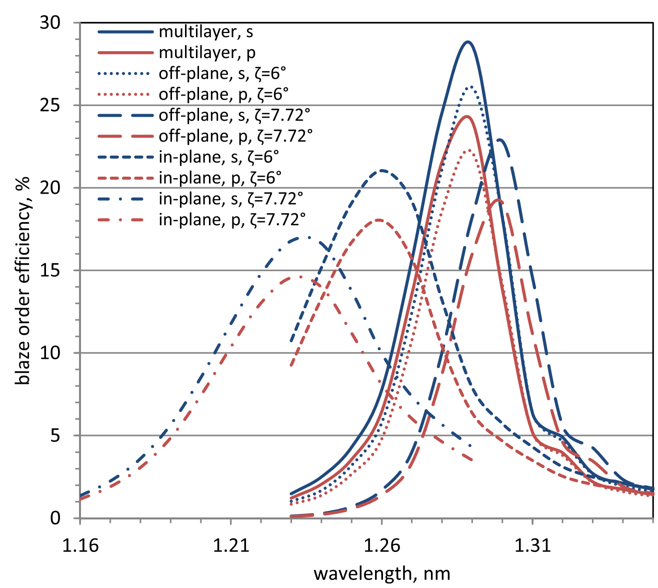

FIG. 3. Spectral s and p dependences of the efficiency of a blazed grating with $d=114.3$ nm and $\zeta=6°$ or $d=200$ nm and $\zeta=7.72°$ coated by 50 W/B_4C symmetrical bilayers.

accordance with Eq. (5) (see in Fig. 3). At the same time, minor narrowing of the efficiency curves occurs in conical diffraction, while for in-plane diffraction a significant broadening exists (see also in Ref. 11). The first factor affecting η is shadowing that is smaller for grazing-incidence off-plane mounts passing light along the grooves. The second factor affecting diffraction efficiency is refraction effects which result in a shift of the efficiency curves in Figs. 2 and 3. A shift of the resonance wavelength and a change of the spectral bandwidth are minor for conical diffraction mounts and significant and more complex—for respective classical mounts (see also in Refs. 11 and 12). The third factor affecting η is absorption that is also higher for in-plane mounts. It is due to enhanced absorption and reduced transparency of a multilayer stack under asymmetrical diffraction which is a key feature of in-plane mounts. Since the absorption length is always longer for asymmetrical diffraction, absorption of a HFMBG is always stronger for in-plane mounts as compared to the corresponding off-plane mounts or multilayers. Absorption of soft x-rays in asymmetric diffraction devices, like as in-plane HFMBGs or asymmetrically cut single crystals, can be reduced by significant shrinking Γ-ratio and/or by choice of less absorbing materials (see in Ref. 11). However, producing high-quality atomic-scale layers of W with $\Gamma \sim 0.1$–0.2 is a difficult task even for flat multilayers.[20] For triangular substrates, the development is much harder due to strong perturbations and collapses of a multilayer structure in the vicinity of anti-blaze facets.[21] Unfortunately, only a few absorbing materials with some technological and reflectance limitations can be considered for this wavelength range.[18]

Off-plane symmetrical diffraction on HFMBGs, in opposite to grazing-incidence in-plane asymmetrical diffraction, mitigates refraction effects, absorption enhancement, weakening of blazing ability, and eventually results in enhancement of η. Moreover, such off-plane efficiency enhancements are higher for higher blazed orders. We found a possibility for conical diffraction and symmetrical multilayer coatings, which are easy to fabricate, to enhance η of soft-x-ray HFMBGs, especially in higher orders, very closely to the absolute limit, i.e., 0.92–0.98 of the reflectance of the respective W/B4C multilayers. The preferable period for any mount is $\sim$100 nm, but d even a few times higher is still effective. The preferable range of ζ is several degrees; however, higher blaze angles are also working. Thus, the use of x-ray HFMBGs in off-plane mounts and high orders is very promising; however, numerical optimization of all the HFMBG and mount parameters is required to reach the maximal η in a desired order. Real boundary and layer parameters of HFMBGs including interface random roughness can be also taken into account rigorously in our model.[14,19,22]

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