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Optical properties of sliced multilayer gratings

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Abstract

Fabrication, calculation and optical properties of gratings fabricated by bevel cutting multilayer structures are discussed. Such gratings have very short period (about 100 nm) and provide high angular dispersion as compared to ruled, holographic or multilayer coated gratings without reduction of diffraction efficiency. Using graded multilayers it is possible to produce sliced multilayer gratings (SMG) with graded period (GSMG), which can focus radiation in one direction. Examples of SMG for various wavelengths in the interval 2–20 nm are considered.

Keywords: Grating; Sliced multilayer; X-ray; Spectroscopy

1. Introduction

One of the important application fields of modern X-ray optics is X-ray spectroscopy, which requires spectral optical elements with high dispersion and high efficiency. In spite of the obvious progress in technology, conventional ruled, holographic and multilayer coated gratings are still restricted by the value of groove density $\sim 5 \times 10^4$ grooves/mm. This paper considers sliced multilayer gratings (SMG), which can be fabricated by cutting multilayer structures at some angle, as a solution of this problem.

The first sliced multilayer gratings based on Mo/Si coatings were created several years ago and have been utilized for acquiring laser plasma spectra in the wavelength range 12–30 nm [1,2]. However, the application field of SMG can be a great deal wider. SMG were proposed for spectroscopy of hard X-rays up to 20 keV [3,4].

SMG inherit from multilayers high diffraction efficiency in the resonant order and very short period (about 100 nm) that leads to high angular dispersion. These remarkable dispersion properties of SMG allow the development of compact spectrometers and polarimeters, which might be useful in plasma spectroscopy, astrophysics, material science and biology.

Slight improvement of technology allows creation of SMG with graded (slowly changing) period. These gratings are able to focus X-ray radiation along one direction providing advanced

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resolution properties without additional optics. The design of SMG has to meet the requirements of a specific application. This paper gives an approach to calculate their diffraction efficiency and working range.

In this paper we consider fabrication, optical properties and calculation methods of SMG and GSMG. New types of SMG for various wavelengths 2–20 nm are discussed. For the first time the diffraction efficiency for s- and p-polarized beams is found.

2. Fabrication of SMG

Fabrication of a sliced multilayer grating includes several stages.

The first stage. A multilayer periodic coating with a large number of periods ($N = 500$–1000) is applied onto a silicon substrate. Deposition technology is similar to one used for fabrication of multilayer X-ray mirrors. As a rule the method of magnetron sputtering is used to form layers. Coating parameters (pair of materials, period, layer thickness ratio, etc.) are optimized to get the highest efficiency in the work wavelength band of the designed diffraction grating.

The second stage. The substrate with the multilayer coating is cut into workpieces of required dimension (3×12 mm^2). Then each workpiece is stuck to the silicon plate of similar dimensions, the multilayer coating being between silicon plates.

The third stage. A bevel cut is conducted by removing a part of the formed sandwich at a grinder. For this purpose the sandwich is fixed in a special holder providing a required tilt of the workpiece to the surface of an abrasive disc.

The fourth stage. Polishing and finishing of the sliced grating surface is carried out at a polishing machine with the application of fine diamond paste during several steps and successive decrease of the size of the abrasive grains.

Eventually the structure (SMG) with N periods shown in Fig. 1 is made. It is evident from this figure that

$$D = d/\sin\alpha, \tag{1}$$

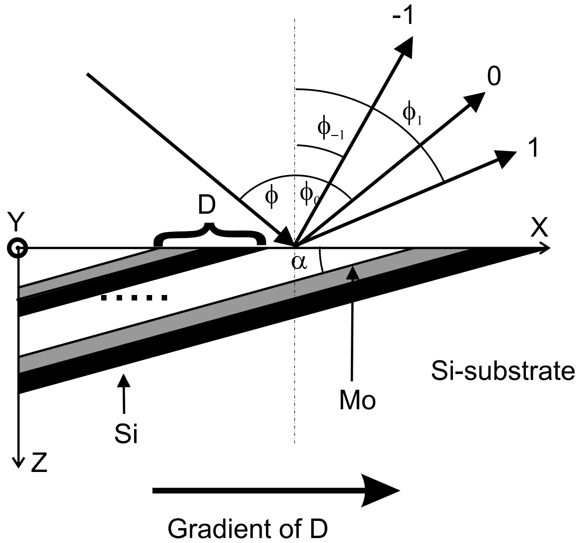

Fig. 1. The scheme of a SMG, where α is slicing angle, D is grating period.

where d is the multilayer period. SMG technology enables creation of gratings that have 10^4 grooves per mm or more.

3. Preliminary consideration of blaze effect in SMG

Any SMG obeys the same general principles as a usual grating. So to determine the angles of diffraction orders, usual grating equation (see [5]) can be used

$$D(\sin\phi_n - \sin\phi) = n\lambda, \quad n = 0, \pm 1, \pm 2, \ldots, \tag{2}$$

where λ is the wavelength, ϕ is an incident angle, ϕ_n are diffraction angles (see Fig. 1) and D is defined by (1).

However SMG can be considered from a different point of view. Since SMG is based on multilayer coating one can expect that the maximum of diffraction efficiency should appear if the multilayer resonant Bragg condition is satisfied. In terms of SMG (see Fig. 1) it can be written as

$$2d\cos(\phi - \alpha) = m\lambda, \quad m = 0, \pm 1, \pm 2 \ldots \tag{3}$$

The beam specularly reflected from the layers has evidently the angle

$$\phi_m = \phi - 2\alpha. \tag{3a}$$

With this formula (3) can be transformed to

$$2d\cos\left(\frac{\phi + \phi_m}{2}\right) = m\lambda, \quad m = 0, \pm 1, \pm 2 \ldots \tag{4}$$

Now it can be shown easily that Eq. (4) with (3a) is equivalent to the grating equation (2). This means that if the incident beam is in Bragg reflection in respect to the layers then the beam specularly reflected from the layers coincides with the mth diffraction order of SMG. This phenomenon is similar to the blaze effect in conventional optics.

The equivalence of (4) (with (3a)) and (2) follows from the identity

$$\cos\left(\frac{\phi + \phi_m}{2}\right) = \frac{\sin\phi - \sin\phi_m}{2\sin(\phi - \phi_m)/2}. \tag{5}$$

Introducing (5) into (4) and taking into account that $\phi - \phi_m = 2\alpha$ (see (3a)) and (1) we obtain grating equation (2). The first diffraction order $m = 1$ is of the main practical importance as the first Bragg reflection peak of a multilayer has usually the highest reflectivity.

In conclusion, to achieve the blaze effect in SMG with a slicing angle α it is necessary to choose the angle of incidence ϕ according to Bragg equation (3) with $m = 1$. Then the first diffraction order is expected to appear with enhanced efficiency and close to specular reflection from the layers.

In this section we gave a qualitative consideration of SMG properties basing on the grating equation (2) and Bragg equation (3). Both can be used to determine the directions of diffraction orders.

4. Solution of wave equation in SMG. An approach to numerical solution

For consistent calculation of diffraction efficiency of SMG the solution of Maxwell equations should be found. Taking into account that in experiment the incident plane is usually perpendicular to the grating grooves (see Fig. 1), any electromagnetic wave can be expressed as a sum of two independent waves with different polarizations: s with electric vector $\vec{E}$ that is perpendicular to incident plane and p with magnetic vector $\vec{B}$ that is perpendicular to the same plane. Diffraction efficiency for each polarization can be calculated separately and the most convenient equations for this purpose are:

$$\Delta_{x,z}E + \varepsilon(x,z)E = 0 \quad \text{for s-polarization and} \tag{6a}$$

$$\Delta_{x,z}B - \frac{\varepsilon'_x}{\varepsilon}\frac{\partial B}{\partial x} - \frac{\varepsilon'_z}{\varepsilon}\frac{\partial B}{\partial z} + k^2\varepsilon B = 0 \quad \text{for p-polarization.} \tag{6b}$$

Here scalar values E and B are the normal components of fields in respect to the incident plane, ε is the dielectric function of medium, k is the wave number. Since the incident plane is perpendicular to the grating grooves and the grating is infinite in y-direction all values in (6a) and (6b) depend only on two spatial coordinates x and z (Fig. 1).

To simplify calculation it is supposed that grating is infinite also in x-direction and therefore it is a periodic structure along this coordinate. The finite size of SMG in x-direction leads only to small corrections due to an additional divergence of diffraction orders. To solve Eqs. (6a) and (6b) each value may be expanded in a Fourier series, which inside SMG are:

$$\varepsilon(x,z) = \sum_{n=-\infty}^{+\infty} \varepsilon_n(z) e^{inx2\pi/D}. \tag{7}$$

$$E = \sum_{n=-\infty}^{+\infty} e^{ikx\sin\phi} e^{-in(2\pi/D)x} f_n(z), \tag{8a}$$

$$B = \sum_{n=-\infty}^{+\infty} e^{ikx\sin\phi} e^{-in(2\pi/D)x} f_n^B(z), \tag{8b}$$

where

$$\varepsilon_n(z) = \frac{\varepsilon_1 - \varepsilon_2}{\pi n}\sin\pi n\beta e^{izn2\pi\cos\alpha}, \quad n \neq 0,$$

$$\varepsilon_0 = \beta\varepsilon_1 + (1-\beta)\varepsilon_2,$$

and ε_i are dielectric functions of multilayer materials, $\beta = d_1/d$, d_1 is the thickness of the most absorptive material in the structure. Providing that incident wave is normalized to unit, Fourier series outside SMG are:

$$E = \sum_{n=-\infty}^{+\infty} e^{ikx\sin\phi} e^{-in(2\pi/D)x} \left(\delta_{0n} e^{ik_z^n z} + R_n e^{-ik_z^n z}\right), \quad (9a)$$

$$B = \sum_{n=-\infty}^{+\infty} e^{ikx\sin\phi} e^{-in(2\pi/D)x} \left(\delta_{0n} e^{ik_z^n z} + R_n^p e^{-ik_z^n z}\right), \quad (9b)$$

where R_n and R_n^p are the diffraction coefficients for s and p polarizations, respectively, and

$$k_z^n = \sqrt{k^2 - n^2\left(\frac{2\pi}{D}\right)^2}.$$

The boundary conditions at the surface of SMG providing continuity of fields and their first derivatives also should be used.

Taking into account (8a) and (8b), Eqs. (6a) and (6b) can be transformed into systems of ordinary differential equations:

$$f_n'' = -k^2 \sum_{m=-\infty}^{+\infty} f_m \left[\varepsilon_{m-n}(z) - \delta_{mn}\left(\sin\phi - \frac{2\pi m}{kD}\right)^2\right], \quad (10a)$$

$$f_n^{B''} = -\sum_{m=-\infty}^{+\infty} \left(\frac{\varepsilon_z'}{\varepsilon}\right)_{m-n} f_m^{B'} - k^2 \times \sum_{m=-\infty}^{+\infty} f_m^B \left[\varepsilon_{m-n}(z) - \delta_{mn}\left(\sin\phi - \frac{2\pi m}{kD}\right)^2 - \frac{i}{k}\left(\frac{\varepsilon_x'}{\varepsilon}\right)_{m-n}\left(\sin\phi + \frac{2\pi m}{kD}\right)\right], \quad (10b)$$

where

$$\left(\frac{\varepsilon_x'}{\varepsilon}\right)_{n\neq 0} = \frac{2i}{D}(\ln\varepsilon_1 - \ln\varepsilon_2)\sin(\pi\beta n)e^{iz(2\pi n/d)\cos\alpha},$$

$$\left(\frac{\varepsilon_x'}{\varepsilon}\right)_{n=0} = 0,$$

$$\left(\frac{\varepsilon_z'}{\varepsilon}\right)_n = \mathrm{ctg}\alpha\left(\frac{\varepsilon_x'}{\varepsilon}\right)_n, \quad n = 0, \pm1, \pm2, \ldots$$

Eqs. (10a) and (10b) are systems of coupled wave equations. They should be solved together with (9a) and (9b), which are actually boundary conditions for $z \to -\infty$. However an additional boundary condition is required. In accordance with general principles of scattering problem inside the SMG, for $z \to +\infty$ the field should propagate only from the surface of SMG.

To simplify further calculations formulas (10a) and (10b) can be expressed in matrix form:

$$\vec{f}'' = -k^2 A\vec{f}, \quad (11a)$$

$$\vec{f}_B'' = S\vec{f}_B' - k^2 A_B \vec{f}_B, \quad (11b)$$

where $\|\vec{f}\|_n = f_n$, $\|\vec{f}_B\|_n = f_n^B$ and

$$\|A\|_{mn} = \varepsilon_{m-n}(z) - \delta_{mn}\left(\sin\phi - \frac{2\pi n}{kD}\right)^2,$$

$$\|A_B\|_{mn} = \varepsilon_{m-n}(z) - \delta_{mn}\left(\sin\phi - \frac{2\pi n}{kD}\right)^2 - \frac{i}{k}\left(\frac{\varepsilon_x'}{\varepsilon}\right)_{m-n}\left(\sin\phi + \frac{2\pi m}{kD}\right),$$

$$\|S\|_{mn} = \left(\frac{\varepsilon_z'}{\varepsilon}\right)_{m-n}.$$

It is convenient to introduce a matrix

$$M = F'F^{-1}, \quad (12)$$

where matrix $F = \|\vec{f}_1 \cdots \vec{f}_n\|$ is a set of vectors. Then equations for M are obtained from Eqs. (11a) and (11b). These equations have the form similar to scalar Rikkaty equation

$$M' = -M^2 - k^2 A, \quad (13a)$$

$$M_B' = -M_B^2 + SM_B - k^2 A_B. \quad (13b)$$

Eqs. (13a) and (13b) can be solved numerically, for instance, by the Runge–Kutta method. During the solution one should take into account boundary condition in infinity ($z \to +\infty$) and also should consider reasonable finite number of equations that provide required accuracy. The detailed discussion of such a method is beyond the scope of this paper. In Section 3 examples of calculations for various wavelength ranges are provided.

After solution of (13a) and (13b) diffraction coefficients R_n and R_n^p should be found. The value of M (or M_B) matrix is now known from the numerical solution. The diffraction coefficients can be calculated taking into consideration boundary conditions at the surface of SMG and expansions (9a) and (9b). The final expressions are:

$$\vec{R} = (\mathrm{i}K + M)^{-1}(\mathrm{i}K - M)\vec{I}, \quad (14a)$$

$$\vec{R}_p = (\mathrm{i}K + TM_B)^{-1}(\mathrm{i}K - TM_B)\vec{I}, \quad (14b)$$

where matrixes M and M_B are taken at the surface of SMG, $\vec{R}$ and $\vec{R}_p$ are vectors of diffraction coefficients and

$$\|K\|_{mn} = \delta_{mn}k_z^n,$$

$$\|\vec{I}\|_n = \delta_{0n},$$

$$\|T\|_{mn} = \left(\frac{1}{\varepsilon}\right)_{m-n},$$

$$\left(\frac{1}{\varepsilon}\right)_{n\neq 0} = \frac{(1/\varepsilon_1) - (1/\varepsilon_2)}{\pi n}\sin(\pi n\beta)\mathrm{e}^{\mathrm{i}zn2\pi\cos\alpha},$$

$$\left(\frac{1}{\varepsilon}\right)_{n=0} = \frac{1}{\varepsilon_1}\beta + \frac{1}{\varepsilon_2}(1-\beta).$$

Formulas (14a) and (14b) resemble Fresnel ones and can be called Fresnel matrix formulas for SMG. Now real diffraction efficiency in the nth order can be expressed by formula

$$r_n^{(p)} = \left|R_n^{(p)}\right|^2 \frac{\cos\phi_n}{\cos\phi} \quad (15)$$

that takes into account geometry of SMG and satisfies energy conservation principle

$$\sum_{n=-\infty}^{n=+\infty} r_n^{(p)} \leqslant 1. \quad (16)$$

In formula (16) equality appears in the case when there is no absorption.

To summarize, for calculation of diffraction efficiencies of SMG for both polarizations one should solve (13a) and (13b) by some numerical method, take M (or M_B) matrix at the surface of SMG and use (14a) and (14b) to calculate diffraction coefficients. The efficiencies are determined using formula (15).

5. The examples of SMG

To illustrate the SMG properties, several examples of SMG in a number of wavelength intervals were calculated. The list of these SMG is given in Table 1.

(a) The first wavelength range is 12–20 nm, where the first samples of SMG were fabricated and tested [1,2]. The most common multilayer structure used here is Mo/Si. This range is of particular interest for astrophysics as contains many important spectral lines. Fig. 2 depicts the first diffraction order efficiencies of $MoSi_2$/Si sliced multilayer grating. This type multilayer structure is characterized by enhanced radiation and heat stability [6] that is important for space optics and free electron lasers. The calculations were performed for both polarizations. One can see that near incidence angle 50° p-polarized radiation is suppressed, which allows to design polarizers for this wavelength interval.

(b) The next example is Mo/ B_4C structure (see Fig. 3). Calculations for p polarization in Figs. 3–5 are not shown because the difference between s and p polarization is negligible.

(c) The third example is Ni/C SMG (see Fig. 4). This wavelength range (4.4–6 nm) is important for biology because of low absorption of radiation in carbon containing materials near the carbon K-edge. So creation of effective spectrometers based on SMG would be a great deal of interest.

Table 1
Sliced multilayer gratings, which efficiencies were calculated in this paper

SMG	d (nm)	β	D (nm)	α (deg)	Wavelengths (nm)
$MoSi_2$/Si	19.5	0.4	112.3	170	12–20
Mo/B_4C	15.5	0.4	89.3	10	6.7–10
Ni/C	10	0.4	57.6	10	4.4–6.0
W/Si	10	0.4	191.1	3	1.5–3.0

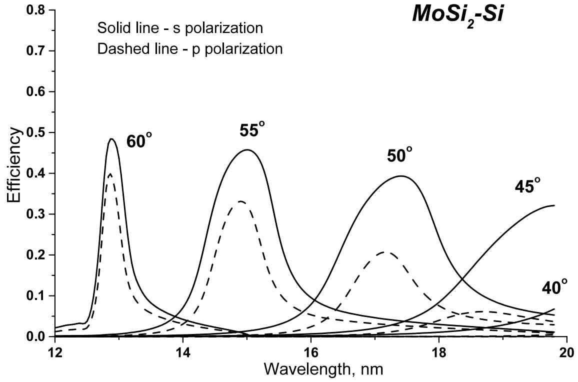

Fig. 2. The first-order efficiencies of $MoSi_2/Si$ SMG (see Table 1) as functions of wavelength at several incidence angles. Both s and p polarizations are depicted.

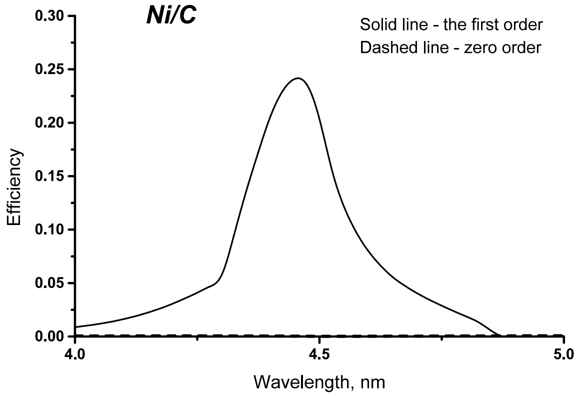

Fig. 4. The first- and zero-order efficiencies of Ni/C SMG (see Table 1) as functions of wavelength for s polarization. The incidence angle is 85°.

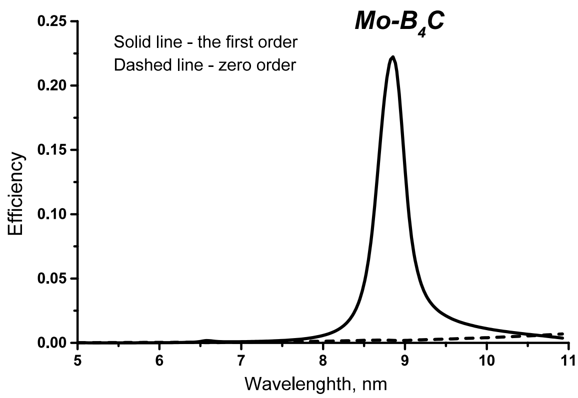

Fig. 3. The first- and zero-order efficiencies of Mo/B_4C SMG (see Table 1) as functions of wavelength for s polarization. The incidence angle is 81°.

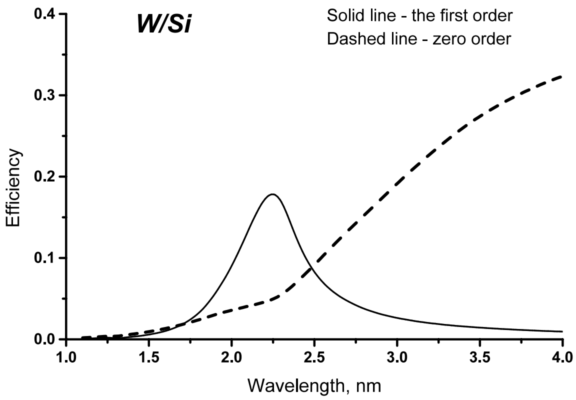

Fig. 5. The first- and zero-order efficiencies of W/Si SMG (see Table 1) as functions of wavelength for s polarization. The incidence angle is 85°.

(d) The last example is W/Si SMG (see Fig. 5). This particular wavelength interval comprises so-called 'water window' where biological objects are transparent for X-ray radiation. So effective spectrometer would be very useful in this spectral range.

The examples given above show that SMG as a new type of spectral devices can enable creation of high efficiency, high dispersion spectral optical elements for the wide wavelength interval 2–20 nm and would be useful in astrophysics, material science and biology.

6. SMG with graded period

The gratings discussed above have a constant period. However during the deposition of a multilayer coating it is possible to introduce slight and monotonic variation of the period. The SMG produced from such a multilayer also has the period changing monotonically and can be called SMG with graded period or graded SMG (GSMG).

The condition that the period is changing slowly in GSMG is essential because it allows simplified description using geometric optics.

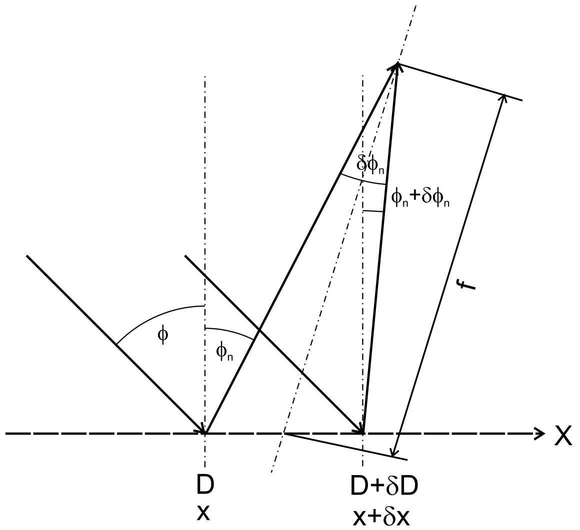

Fig. 6. Focusing X-ray radiation using GSMG.

Basically GSMG works as a cylindrical lens focusing X-ray beam in dispersion plane. The condition of applicability of this simplified model is

$$\left|\frac{D_1 - D_N}{D_1}\right| \ll 1. \quad (17)$$

Here D_1 is the first period of the GSMG; D_N is the last period of GSMG. Condition (17) means that the change of period over the whole grating should be small as compared with period itself.

To calculate focus distance of GSMG (see Fig. 6) we suppose that period D is continuous function of coordinate x. Considering two points with coordinates x and $x + \delta x$ (see Fig. 6) the angle difference $\delta\phi_n$ can be obtained from Eq. (2)

$$\delta\phi_n = -\frac{\delta D}{D}\frac{\lambda}{D}\frac{n}{\cos\phi_n}. \quad (18)$$

From Fig. 6 it is obvious that

$$f = \delta x\frac{\cos\phi_n}{\delta\phi_n}.$$

The final expression for focus distance is

$$f = -\frac{D^2}{n\lambda\gamma}\left[1 - \left(\sin\phi + \frac{n\lambda}{D}\right)^2\right], \quad \gamma = \frac{\delta D}{\delta x}. \quad (19)$$

For a GSMG with typical parameters: $D = 112$ nm, $\lambda = 15$ nm, $n = 1$, $\sin\phi = 0.77$ ($\phi = 50°$), $\gamma = -2 \times 10^{-4}$ the focus distance $f = 2.48$ cm, which is quite a short one.

7. Summary

In this paper sliced multilayer gratings (SMG) as a new type of spectral dispersion devices for soft X-ray radiation were discussed. The efficiency of SMG with the account for polarization of incident beam is firstly calculated. The results show that SMG can be used to construct X-ray spectrometers with high dispersion and diffraction efficiency. In spite of relatively narrow spectral band SMG can be useful when one need to resolve many spectral lines crowded in narrow spectral range (for example, it is often the case in Solar spectrum). Such spectrometers can work in wide wavelength range 2–20 nm and can be used to solve various problems in biology, astrophysics, material science, etc. In the long wavelength part of this spectral interval they also can be utilized as effective polarizers.

Sliced multilayer gratings with graded period (GSMG) were also considered. They provide focusing of the spectra and can be used in imaging spectrometers.

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