Quantum Electronics **35** (2) 195 – 199 (2005)

PACS numbers: 07.85.Fv
DOI: 10.1070/QE2005v035n02ABEH003728

Algorithm for calculating the optimal parameters of multilayer aperiodic mirrors for soft X-rays

D.S. Burenkov, Yu.A. Uspenskii, I.A. Artyukov, A.V. Vinogradov

Abstract. **A new algorithm is proposed for optimising the thickness of layers in multilayer aperiodic mirrors. An important feature of the algorithm is the separation of the explicit dependence of the reflection coefficient on the thickness of one layer. This reduces the amount of calculations required for the mirror optimisation by a factor of N (N is the number of layers of the mirror). The algorithm allows one to perform optimisation of different types: the obtaining of the maximum reflection coefficient at one frequency, the maximum of the integrated reflection coefficient within a specified frequency interval, the constant reflection coefficient in the working frequency or angular interval, etc. Examples of practical applications of the algorithm demonstrating its efficiency and versatility are presented.**

Keywords: *multilayer aperiodic mirrors, algorithm for optimising parameters, soft X-ray range.*

1. Introduction

Multilayer X-ray mirrors are widely used as reflecting and focusing elements in X-ray optics and to control soft X-ray beams [1 – 3]. The complex refractive index $n = 1 - \delta + i\beta$ for all materials in the soft X-ray range is close to unity, resulting in the weak reflection of X-rays from one surface. To increase the reflection coefficient, the interference of the waves reflected from several interfaces is used. A typical multilayer coating has a few tens and even hundreds of alternating layers of two materials, providing the reflection coefficient achieving a few tens of percent [1, 2].

Many practical applications require mirrors having not only the high reflection coefficient at a certain wavelength but also the maximum integrated reflection coefficient in a broad spectral range. Such mirrors can be fabricated by using aperiodic multilayer coatings in which the layer thickness changes with depth. The thickness of layers is usually selected to minimise some estimating function. However, a great number of variables and a complicated profile of this function make the solution of this problem with the help of standard mathematical methods extremely time-consuming.

Many attempts have been made to overcome these difficulties and to develop the efficient optimisation algorithms. For this purpose, the methods successfully used in the development of mirrors for neutron beams were employed [4], and the genetic algorithm was proposed [5]. The algorithm proposed in [6] is based on the single-pass optimisation of mirror layers. In [7], chirped mirrors were fabricated by using successively added very thin (acicular) layers, and X-ray mirrors were designed in [8, 9] by employing the explicit expression for calculating derivatives and the method of gradient descent for the search for a maximum. In [10], the analytic expressions for the reflection coefficient were obtained with the help of the quasi-classical approximation, which were used in the development of optimal multilayer mirrors. In [11], the dependence of the reflection coefficient on the layer thickness was analysed in detail and a comparatively simple expression was obtained for the initial approximation, thereby considerably increasing the optimisation rate of mirror layers.

We developed a new method that allows the separation of the explicit dependence of the reflection coefficient on the thickness of one layer. This considerably reduces the amount of calculations, expands the region of search for the extremum, and allows the optimisation of the layer thickness in many problems of the soft X-ray optics.

2. Basic formulas

In this paper, we consider coatings consisting of alternating plane – parallel layers of two materials. The complex amplitude reflection coefficient $r(\lambda, \theta)$ of such a structure can be calculated with the help of recurrence relations [1]

$$r_k = \frac{r_k^{\mathrm{F}} + r_{k+1}\mathrm{e}^{2\mathrm{i}\beta_{k+1}}}{1 + r_k^{\mathrm{F}} r_{k+1}\mathrm{e}^{2\mathrm{i}\beta_{k+1}}},$$

$$r(\lambda, \theta) = r_{k=0}, \tag{1}$$

$$r_{N+1} = 0,$$

where $\beta_k = (2\pi/\lambda_0)h_k(n_k^2 - \sin^2\theta)^{1/2}$; N is the number of mirror layers; r_k^{F} is the Fresnel amplitude reflection coefficient for the kth interface (between kth and $k+1$th layers); n_k is the complex refractive index of the kth layer; λ_0 is the radiation wavelength incident on the multilayer

D.S. Burenkov, Yu.A. Uspenskii, I.A. Artyukov, A.V. Vinogradov
P.N. Lebedev Physics Institute, Russian Academy of Sciences, Leninskii prosp. 53, 119991 Moscow, Russia; e-mail: vinograd@sci.lebedev.ru

Received 24 December 2003; revision received 13 October 2004
Kvantovaya Elektronika **35** (2) 195 – 199 (2005)
Translated by M.N. Sapozhnikov

coating from vacuum at an angle of θ. Similar relations for the complex amplitude transmission coefficient $t(\lambda, \theta)$ have the form

$$t_k = \frac{t_{k+1} t_k^{\mathrm{F}} \mathrm{e}^{\mathrm{i}\beta_k}}{1 + r_k^{\mathrm{F}} r_{k+1} \mathrm{e}^{2\mathrm{i}\beta_k}},$$

$$t(\lambda, \theta) = t_{k=0}, \qquad (2)$$

$$t_{N+1} = 1.$$

The problem of optimising a multilayer reflection coating is solved, as a rule, by finding the extremum of the corresponding objective function of $r(\lambda, \theta, \{h\})$ in the multidimensional space $\{h\}$ determined by a set of thicknesses of layers in this coating. The search for such an extremum in most numerical algorithms is performed by using successive approximations, each of these approximations (hereafter, referred to as a step) requiring the iterative passage over the coordinates of the multidimensional space. Moreover, by optimising the mirror characteristics in the specified wavelength or angular range, it is necessary to calculate the coefficients $r(\lambda, \theta, \{h\})$ at many points on the axis λ or θ (the number of points is determined by the form of the objective function and the number of oscillations of the reflection curve in this range). In the case of the integral objective function (for example, the maximum integrated reflection coefficient), the influence of fast oscillations is weak and the choice of the number of points is insignificant. In this case, the time of calculations performed by (1) is proportional to $N^2 I$, where $N \sim 50 - 400$, and I is the number of steps, which depends on the method of search for an extremum and the required accuracy. When it is necessary to make the reflection curve as close as possible to the specified dependence, oscillations make a substantial contribution to the objective function. To take them into account, a rather fine integration grid with the number of points proportional to N should be used. In this case, the amount of calculations performed by (1) can be estimated as $\sim N^3 I$.

To reduce the amount of calculations, it is convenient to separate the explicit dependence of $r(\lambda, \theta, \{h\})$ on the thickness of one layer. For this purpose, we divide a multilayer mirror into three parts: the multilayer structure between vacuum and the kth layer (denoted by the subscript 'a'), the kth layer itself, and the multilayer structure between the kth layer and a substrate (subscript 'b'). In this case, the required reflection coefficient can be represented in the form [12]

$$r = r_{\mathrm{a}} + \frac{t_{\mathrm{a}} \tilde{t}_{\mathrm{a}} r_{\mathrm{b}} \mathrm{e}^{2\mathrm{i}\beta_k}}{1 - r_{\mathrm{b}} \tilde{r}_{\mathrm{a}} \mathrm{e}^{2\mathrm{i}\beta_k}}, \qquad (3)$$

where r_{a}, r_{b}, and t_{a} are the reflection and transmission coefficients of the corresponding structures in the forward direction, and $\tilde{r}_{\mathrm{a}}$ and $\tilde{t}_{\mathrm{a}}$ in the backward direction. Thus, we separated explicitly the dependence of $r(\lambda, \theta)$ of the thickness of the kth layer, and now the selection of the thickness of this layer in any numerical algorithm is substantially simplified. Moreover, to calculate the dependence of $r(\lambda, \theta)$ on the thickness of the $(k+1)$ layer, there is no need to recalculated all the reflection coefficients entering (3). They can be calculated with the help of iterative expressions

$$r_{\mathrm{b}}(k+1) = \frac{r_k^{\mathrm{F}} - r_{\mathrm{b}}(k)}{[r_{\mathrm{b}}(k) r_k^{\mathrm{F}} - 1]\mathrm{e}^{2\mathrm{i}\beta_k}},$$

$$\tilde{r}_{\mathrm{a}}(k+1) = \frac{r_k^{\mathrm{F}} + \tilde{r}_{\mathrm{a}}(k) \mathrm{e}^{2\mathrm{i}\beta_k}}{1 - r_k^{\mathrm{F}} \tilde{r}_{\mathrm{a}}(k) \mathrm{e}^{2\mathrm{i}\beta_k}},$$

$$\tilde{t}_{\mathrm{a}}(k+1) = \frac{\tilde{t}_{\mathrm{a}}(k) t_k^{\mathrm{F}} \mathrm{e}^{\mathrm{i}\beta_k}}{1 - r_k^{\mathrm{F}} \tilde{r}_{\mathrm{a}}(k) \mathrm{e}^{2\mathrm{i}\beta_k}}, \qquad (4)$$

$$r_{\mathrm{a}}(k+1) = r_{\mathrm{a}}(k) + \frac{t_{\mathrm{a}}(k) \tilde{t}_{\mathrm{a}}(k) r_k^{\mathrm{F}} \mathrm{e}^{2\mathrm{i}\beta_k}}{1 - r_k^{\mathrm{F}} \tilde{r}_{\mathrm{a}}(k) \mathrm{e}^{2\mathrm{i}\beta_k}},$$

$$t_{\mathrm{a}}(k+1) = \frac{t_{\mathrm{a}}(k) t_k^{\mathrm{F}} \mathrm{e}^{\mathrm{i}\beta_k}}{1 - r_k^{\mathrm{F}} \tilde{r}_{\mathrm{a}}(k) \mathrm{e}^{2\mathrm{i}\beta_k}}.$$

The use of expressions (3) and (4) eliminates the necessity of calculating $r(\lambda, \theta, \{h\})$ from (1) upon the iterative passage through mirror layers and also allows the analytic calculation of partial derivatives of any orders due to the separation of one of the variables. This approach is versatile and can be used in many methods for searching for the extremum of functions of $r(\lambda, \theta, \{h\})$.

The layer boundaries in expressions (3) and (4) are assumed ideally smooth. When the roughness of interfaces between the layers is substantial, it can be taken into account by multiplying the reflection coefficient by the Debye–Waller factor. Such a simplified description, corresponding to the completely correlated behaviour of the roughness parameter σ on the boundaries of all the layers, preserves the above-described optimisation procedure of multilayer structures also for $\sigma \neq 0$.

As a whole, the algorithm looks as follows. At the first stage, the best parameters of a periodic mirror are determined by a direct sorting. The thicknesses of the layers of this mirror are used as the initial parameters in the method of coordinate descent. Then, this algorithm is used to calculate successively the thicknesses of layers of an aperiodic mirror, which optimise the objective function. Because a set of coefficients r_{a}, r_{b}, t_{a}, $\tilde{r}_{\mathrm{a}}$, and $\tilde{t}_{\mathrm{a}}$ changes during calculations, the thickness selection procedure passes many times through the layers to the point of complete self-consistence (i.e., when the thicknesses of the layers no longer change).

We used the method of coordinate descent for the two reasons. First, due to the separated explicit dependence over each coordinate [see expression (3)], we can compare the depth of several extrema, which is impossible when local methods are used such as the method of gradient descent. Second, the use of expressions (4) reduces the computation time by a factor of N. Therefore, despite a number of disadvantages of the method of coordinate descent [13, 14], this method together with the expressions presented above allow us to construct the efficient algorithm for optimisation of multilayer coatings.

3. Calculation of aperiodic mirrors

We used the algorithm considered above for the search for the optimal parameters of aperiodic coatings satisfying different requirements. The different requirements lead to the difference in the selection of the objective function, whose extremum should be found in a given problem. In particular, to obtain the maximum peak reflection coefficient, it is necessary to find the maximum of the function $F_0 = R(\lambda)$ [where $R(\lambda)$ is the reflection coefficient of the mirror at the specified wavelength λ].

The problem of obtaining the maximum integrated reflection coefficient in the working wavelength or angular range is solved by searching for the maximum of the objective function $F_1 = \int_{x_1}^{x_2} R(x)\mathrm{d}x$, where x_1 and x_2 are the limits of integration over the wavelength or angle. The maximum of this integral does not warrant, however, that the dependence $R(x)$ will not have strong dips. Such dips (as a rule, undesirable) can be eliminated by requiring that the objective function $F_2 = \int_{x_1}^{x_2} [R(x) - R_0]^2\mathrm{d}x$, will have a minimum, which provides the minimum deviation of $R(x)$ from the specified value R_0, but does not warrant the achievement of a large integrated reflection coefficient. To avoid the disadvantages of these two approaches, a more general criterion is required, which would include the combination of these two requirements. The first requirement (the maximum of the integrated reflection coefficient) can be replaced by the condition of the function minimum $F = -\bar{R}^2$, where $\bar{R} = (x_2 - x_1)^{-1} \times \int_{x_1}^{x_2} R(x)\mathrm{d}x$, while the second requirement (the minimum of deviation from the man value) – by the condition of the minimum of the function $\int_{x_1}^{x_2}[R(x) - \bar{R}]^2\mathrm{d}x$. The combination of these requirements leads to the requirement of the minimum of the objective function

$$F_3 = \int_{x_1}^{x_2} \{[R(x) - \bar{R}]^2 - \alpha\bar{R}^2\}\mathrm{d}x, \qquad (5)$$

where the choice of the coefficient α is determined by the relative importance of the two above conditions.

The choice of the region for extremum searching and of the initial approximation is important for most numerical algorithms of optimising functions of many variables [13]. Let us discuss this question in more detail. The main criterion for the choice of the initial point is its proximity to the global extremum (minimum or maximum, depending on the specific problem). Such an extremum in the absence of absorption for a monochromatic wave is the well-known periodic solution. Therefore, in the case of weak absorption (which is fulfilled in the soft X-ray region) and a narrow wavelength or angular region, such a periodic solution will be a good initial approximation. In our calculations, we always used a periodic solution as the initial approximation.

Let us present some theoretical considerations concerning the choice of the region for extremum searching for the objective functions F_1, F_2, and F_3, which allow one to perform the best choice, thereby increasing the algorithm efficiency. It is well known that in the absence of absorption, the increase in the layer thickness by $\lambda/2$ does not change the reflection coefficient at the wavelength λ [15]. This statement is qualitatively correct for soft X-rays as well, because the absorption coefficient of all materials in this spectral region is very small. At the same time the change in the layer thickness by $\lambda/2$ affects the reflection coefficient at wavelengths different from λ. Consider, for example, the dependence of the integrated reflection coefficient on a multilayer Si/Mo coating on the thickness of one layer (Fig. 1). One can easily see that the global maximum of this dependence differs from the extremum at the minimum layer thickness and from the extremum near $\lambda = \lambda_0/4$ (λ_0 is the middle of the integration interval). The consideration of several successive extrema in practice allows one to improve the results in the case when the behaviour of the reflection

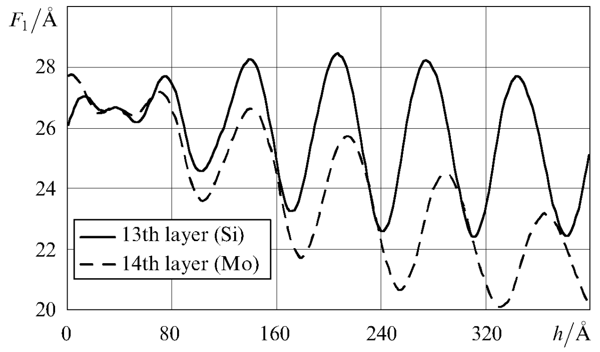

Figure 1. Dependences of the integrated reflection coefficient F_1 on the thickness h of a single layer for the structure consisting of 45 pairs of the Si/Mo layers. The integrated reflection coefficient was determined in the range from 125 to 145 Å.

coefficient is optimised in a broad wavelength or angular range.

We consider below several examples of optimisation of the parameters of multilayer mirrors with the help of this algorithm. The number of layers in the multilayer structure in all the examples was sufficiently large, so that its small variations virtually did not affect the results of optimisation. The values of the optical constants of materials used to calculate the reflection coefficient were taken from [16]. To control the quality of the solutions obtained, we used them as the initial solutions for optimising with the help of the simplex method. Such an optimisation did not provide any improvement in the physically allowed region of parameters for all examples.

Figure 2a shows the reflection coefficient of a multilayer Si/Mo mirror designed to obtain the maximum integrated reflection coefficient in the wavelength between 130 and 180 Å. The optimal thicknesses of the layers are shown in Fig. 2b. The integrated reflection coefficient of this aperiodic mirror is larger by 51.9 % than that of the periodic multilayer coating. Note that the advantage in the integrated reflection coefficient provided by the aperiodic structure for different mirrors is 10 % – 60 %, depending on the wavelength region and materials. The broader the wavelength range, the more significant the advantage. The results for the peak reflection coefficient are much more modest, the increase in the reflection coefficient not exceeding 1 % – 3 %.

Figure 3a compares the reflection coefficients for two Si/Mo structures obtained after optimisation of the objective function F_2 and F_3, respectively, in the range from 135 to 185 Å. One can clearly see that the function F_2 provides a more uniform spectral characteristic, while the function F_3 gives a higher mean reflection coefficient due to a greater deviation of the spectral characteristic from this mean value.

Some X-ray optics systems such as the Schwarzschild objective often require mirrors with a constant reflection coefficient in the specified angular range. Figure 4 demonstrates the calculation of such a mirror for the C/Co pair and the angular range from 4.3° to 9° with the help of our algorithm. Figure 4a compares the reflection coefficients for this and periodic structures realising the same conditions. One can see that a better uniformity of the reflection coefficient is achieved due to a decrease in its absolute value. The optimal thicknesses of Co layers change rather

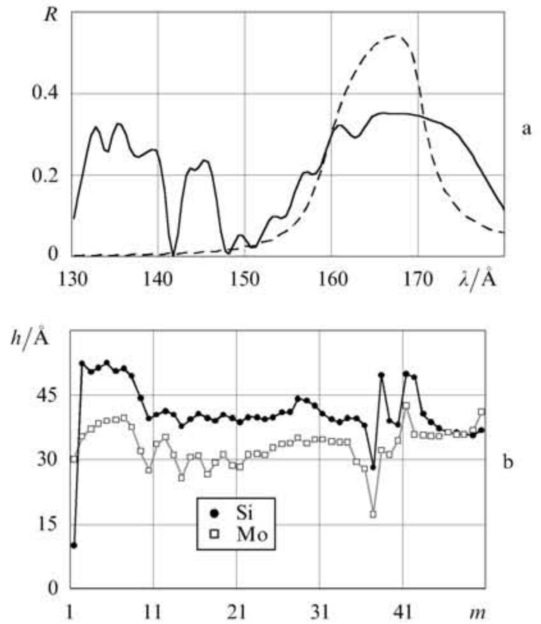

Figure 2. Reflection coefficients R of the periodic (dashed curve) and aperiodic (solid curve) mirrors consisting of 45 pairs of the Si/Mo layers and realising the maximum of the integrated reflection coefficient in the range from 130 to 180 Å (a), and the thickness h of the layers of the aperiodic mirror (here and in Figs 3 and 4, m is the pair number) (b). The advantage on passing to the aperiodic structure is 51.9 %.

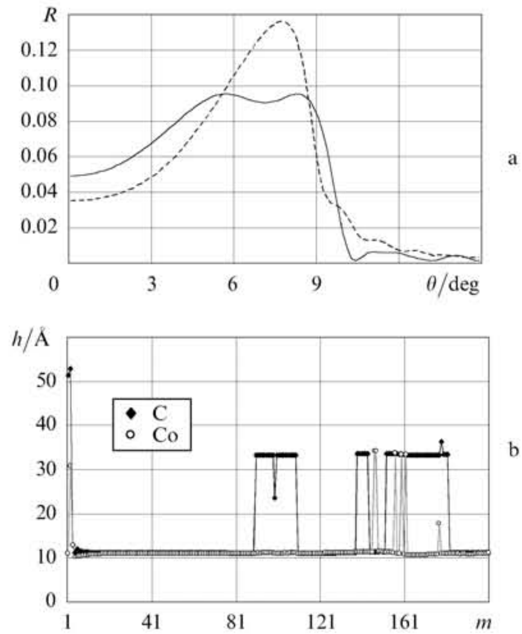

Figure 4. Angular dependences of the reflection coefficients R of the periodic (dashed curve) and aperiodic (solid curve) mirrors realising the minimum of the objective function F_2 for 200 pairs of the C/Co layers in the range of angles of incidence from 4.3° to 9° for $\lambda = 45$ Å (a), and the thickness h of the layers of the aperiodic mirror (b) for $R_0 = 0.3$ and the roughness parameter $\sigma = 4.6$ Å.

weakly with increasing the pair number, whereas the thicknesses of carbon layers have two characteristic values, 11 and 33 Å (Fig. 4b).

We would like to say a few words about the uniqueness of the solution of the problem of optimal design of multilayer X-ray mirrors. Theoretical considerations and calculations show that the objective function always has, except the global minimum, many local minima of different depths. Some of them are very close in depth to the absolute minimum, so that the structures corresponding to them can be also considered optimal from the practical point of view. Our optimisation method uses expression (3), which gives the explicit dependence of the reflection coefficient on the thickness of one layer, for example, h_k. This allows us to consider the behaviour of the objective function in a broad range of variation of h_k and to select the deepest minimum over this variable, omitting shallower minima. Although this procedure (as any of the procedures available at present) cannot warrant the achievement of the absolute minimum because of a great number of variables and a complicated profile of the objective function, it allows one to find a rather deep minimum, which is sufficient for the design of a multilayer structure satisfying the practical requirements.

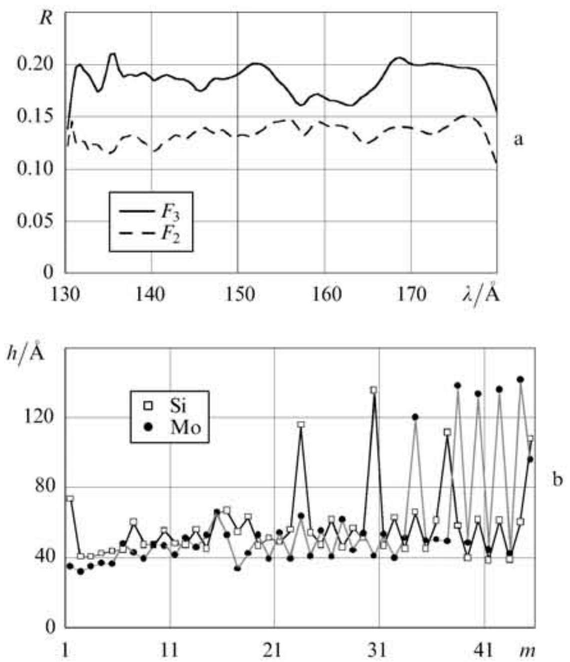

Figure 3. Reflection coefficient R of aperiodic mirrors realising the minimum of the objective functions F_2 and F_3 for 45 pairs of the Si/Mo layers in the range from 135 to 185 Å (a), and the thickness h of the layers of the aperiodic mirror realising the minimum of F_2 (b) for $R_0 = 0.15$ and $\alpha = 0.5$.

Let us present the data characterising the fast operation of the software based on our algorithm. The software was used with a 1.8-GHz Pentium 4 processor. The calculation time T of the reflection coefficient for a multilayer structure containing about 100 layers was 4 ms, while the total calculation time ($\sim TN^2I/100$) was from 3 to 100 s.

4. Conclusions

The optimisation of aperiodic multilayer reflecting coatings is reduced to the determination of the extremum of the function of many variables, which has a complicated profile. The solution of this problem by standard mathematical methods requires a very great amount of calculations. In this paper, we have presented the algorithm that allows the separation of the explicit dependence of the reflection coefficient on the thickness of one layer. This have reduced the amount of calculations by a factor of N and allowed us to perform calculations for multilayer structures having up to 400 layers. Another advantage of our algorithm is its versatility, i.e., its independence of the specific optimisation problem. The algorithm has been successfully used to search the maxima of the peak and integrated reflection coefficients and to solve the inverse problem of finding the configuration of a mirror with the specified spectral characteristic. In the process of the algorithm development, we considered the general question of the choice of the region for extremum searching. Our calculations have shown that in the optimisation problems with a broad working wavelength or angular range, the deeper minima of the objective function are obtained when the thickness of a part of layers is increased by a factor of three. There is good reason to believe that this algorithm can be efficiently used in many problems of soft X-ray optics.

Acknowledgements. The authors thank Yu.S. Kas'yanov for useful discussions. This work was supported by the Russian Foundation for Basic Research (Grant Nos 03-02-16438a, 04-02-17349), ISTC (Grant No. 2297), CRDF (Grant No. RP2-2326-MO-02), and the Integration Program (Grant Nos I0859, V0056).

References

1. Vinogradov A.V., Brytov I.A., Grudskii A.Ya., Kogan M.T., Kozhevnikov I.P., Slemzin V.A. *Zerkal'naya rentgenovskaya optika* (X-ray Mirror Optics) (Leningrad: Mashinostroenie, 1989).
2. Vinogradov A.V. *Kvantovaya Elektron.*, **32**, 1113 (2002) [*Quantum Electron.*, **32**, 1113 (2002)].
3. Kuhlmann T., Yulin S., Feigl T., Kaiser N. *Proc. SPIE Int. Soc. Opt. Eng.*, **4782**, 196 (2002).
4. Joensen K.D. *Proc. SPIE Int. Soc. Opt. Eng.*, **3113**, 500 (1997).
5. Allred D.D., Turley R.S., Squires M.B. *Proc. SPIE Int. Soc. Opt. Eng.*, **3767**, 280 (1999).
6. Yamamoto M., Namioka T. *Appl. Opt.*, **31**, 1622 (1992).
7. Tikhonravov A.V., Trubetskov M.K., Protopopov V.V., Voronov A.V. *Proc. SPIE Int. Soc. Opt. Eng.*, **3738**, 248 (1999).
8. Kolachevsky N.N., Pirozhkov A.S., Ragozin E.N. *Kvantovaya Elektron.*, **30**, 428 (2000) [*Quantum Electron.*, **30**, 428 (2000)].
9. Pirozhkov A.S. *Cand. Diss.* (Moscow: MFTI, 2002).
10. Vinogradov A.V., Feschenko R.M. *Nucl. Instrum. Res. A,* **448**, 142 (2000).
11. Kozhevnikov I.V., Bukreeva I.N., Ziegler E. *Nucl. Intrum. Res. A*, **460**, 424 (2001).
12. Uspenskii Yu.A., Seely J.F., Popov N.L., Vinogradov A.V., Pershin Yu.P., Kondratenko V.V. *J. Opt. Soc. Am. A,* **21** (2), 298 (2004).
13. Kalitkin N.N. *Chislennye metody* (Numerical Methods) (Moscow: Nauka, 1978).
14. Gill P.E., Murray W., Wright M.H. *Practical Optimization* (London: Academic Press, 1981; Moscow: Mir, 1985).
15. Born M., Wolf E. *Principles of Optics* (Oxford: Pergamon Press, 1969; Moscow: Nauka, 1973).
16. Henke B.L., Gullikson E.M., Davis J. *At. Data Nucl. Data Tables,* **54**, 181 (1993); http://www-cxro.lbl.gov.