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Depth-graded multilayer X-ray optics with broad angular response

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Abstract

A method of designing depth-graded multilayer structures with broad angular response for use as coatings in X-ray optics is presented. The design is based on the well-known Fresnel equations and recursive calculation, combined with a merit function plus random variation of the thickness of each layer. This allows the design of multilayer films for different requirements in X-ray optics. Results are presented on the layer thicknesses in depth-graded W/C multilayer films and their reflectivity as a function of the grazing incidence angle for Cu Kα radiation. The required minimum number of bilayers in depth-graded multilayer films depends on the grazing incidence angle, i.e., the saturation effect observed in the design of periodic multilayer films also emerges in the design of depth-graded multilayers. The predicted performances of multilayers designed using this method are superior to those designed using existing methods.

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1. Introduction

Recent years have seen considerable progress in the design of depth-graded X-ray multilayer films which can provide broad wavelength response for grazing incidence X-ray mirrors, as used in a variety of applications including synchrotron radiation, medical optics and, in particular, for space-borne X-ray telescopes [1,2]. There has also been some work on depth-graded multilayer structures with broad angular response, which in principle are easier to model as, with a fixed wavelength, the refractive and absorption indices are constant. Typically, the angular range for efficient reflection of periodic multilayers is less than 0.05° for Cu Kα radiation ($\lambda = 0.154$ nm). In some applications, a wide angular response is desirable, e.g., X-ray telescopes, collimators and scanners [3,4].

In depth-graded X-ray multilayer structures, the layer thickness varies with depth, in contrast to periodic multilayers, so that the different layer pairs can be turned to different angles, thus increasing the angular response. In some cases it is possible to use

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approximations to calculate the design of such depth-graded multilayers in a semi-analytic way [4].

Broadband multilayer films were first discussed for the visible spectrum in 1966 [5] and the approach was applied to thermal neutron optics in the mid 1970s [6,7]. Disregarding absorption in the layers (which is valid for neutron optics), Mezei [6] concluded that continuous reflectivity could be obtained if the thicknesses of the bilayers are determined by

$$d_i = \frac{d_c}{i^{0.25}} \tag{1}$$

where i is the bilayer number counted from the top, d_i is the thickness of the ith bilayer and d_c is the bilayer thickness required for optimum reflectivity at the critical angle or energy. Dedicated design approaches were proposed subsequently [8–10] but none of them considered the effects of absorption in the layers, important for X-ray multilayers, or imperfect layer interfaces. It was first suggested that broadband X-ray multilayers might improve X-ray telescope performance above 10 keV in 1992 [11]. Since then several theoretical and experimental approaches for designing broadband X-ray multilayers have been proposed [12–15]. In particular, Joensen et al. [14] thoroughly investigated the existing approaches for designing broadband neutron optics and compared these with the method of Joensen and co-workers [12,13] in which the bilayer thicknesses are given by the power law expression

$$d_i = \frac{a}{(b+i)^c}\,. \tag{2}$$

Here a and c are positive constants and b is greater than -1. This was found to provide good solutions in specific cases. Another approach is to define a series of constant thickness blocks [1]. In this the five thickest layers, at the top of the stack, are graded, and then there are three sets of layers with constant bilayer thicknesses in each set. The method yields a multilayer design with an approximate power law distribution of the thicknesses.

In the current paper a general method for designing depth-graded multilayer films is described. In this way, it is found that the reflectivity saturation observed in periodic multilayer film designs also emerges for depth-graded multilayers. This shows that there is a minimum number of bilayers needed in such multilayers. Therefore, the task in the design of depth-graded multilayers is first to look for this minimum. A technique for optimising depth-graded multilayer structures to obtain application dependent reflectivity responses then follows.

2. Design model

The performances of depth-graded X-ray multilayer films can be calculated numerically with reasonable precision using the well-known recursive methods based on the Fresnel formulae, so long as the thickness of each layer in the film is known. However, a major point of interest is the inverse problem, i.e., the calculation of the thicknesses of the layers which provide the best approximation to the required shape of the reflectivity curve as a function of grazing incidence angle. From the mathematical point of view, this is a typical variational problem which can be solved by a suitable optimisation method, again recursively and based on the Fresnel equations. However, it is often necessary not only to optimise the shape of the reflectivity curve, but also to make the average reflectivity as high as possible. In addition, in the hard X-ray region interfacial roughness can severely reduce the specular reflectivity of depth-graded multilayers. Thus, the roughness must be included in the calculations. The simplest way to model the effects is to use the standard analysis based on the Debye theory. Assuming that the mean position of a layer boundary is not altered by the roughness, the amplitude of the reflectance at the jth interface is reduced by a factor

$$D_j = \exp\left[-\frac{1}{2}\left(\frac{4\pi\sigma_j \sin\theta_j}{\lambda_j}\right)^2\right] \tag{3}$$

where σ_j is the root mean square value of the effective roughness and θ_j is the grazing incidence angle.

In the method used, the thickness of each layer in the multilayer film is changed randomly in a finite range according to

$$d = d_0(1 + AR) \tag{4}$$

where $R \in [-1,1]$ are random numbers uniformly distributed between -1 and 1 and A is a proportionality factor. A change which results in an improvement, according to a merit function defined below, is accepted by the computer program written to implement the method, otherwise it is rejected. The program uses optical constants determined from the atomic scattering factors available on the Internet [16].

In a similar fashion to many optimisation methods, a numerical measure (the merit function) is needed to minimise undesired features in the reflectivity response of depth-graded multilayers, in order to ensure that the optimisation generates the most desirable structure. Many functional forms can be chosen for this merit function, each representing a particular desired reflectivity curve shape. Because of the complicated relationship between reflectivity and film thickness, optimisation of the merit function is accomplished by taking numerical derivatives and changing the film thickness according to Eq. (4). For example, the merit function can be defined in terms of the form of the reflectivity curve which gives the maximum integrated reflectivity in a desired angle range. Alternatively, the measure which gives an approximately constant reflectivity at the highest obtainable value over the required angular range can be chosen. Whatever merit function is chosen, the thickness of each layer is allowed to change during the optimisation process, but the number and composition of the layers do not change during the optimisation for the results presented here.

Several calculations have been performed for W/C multilayers with a working wavelength of 0.154 nm, i.e., Cu Kα radiation. In each case, the initial multilayer stack was periodic, and a satisfac-

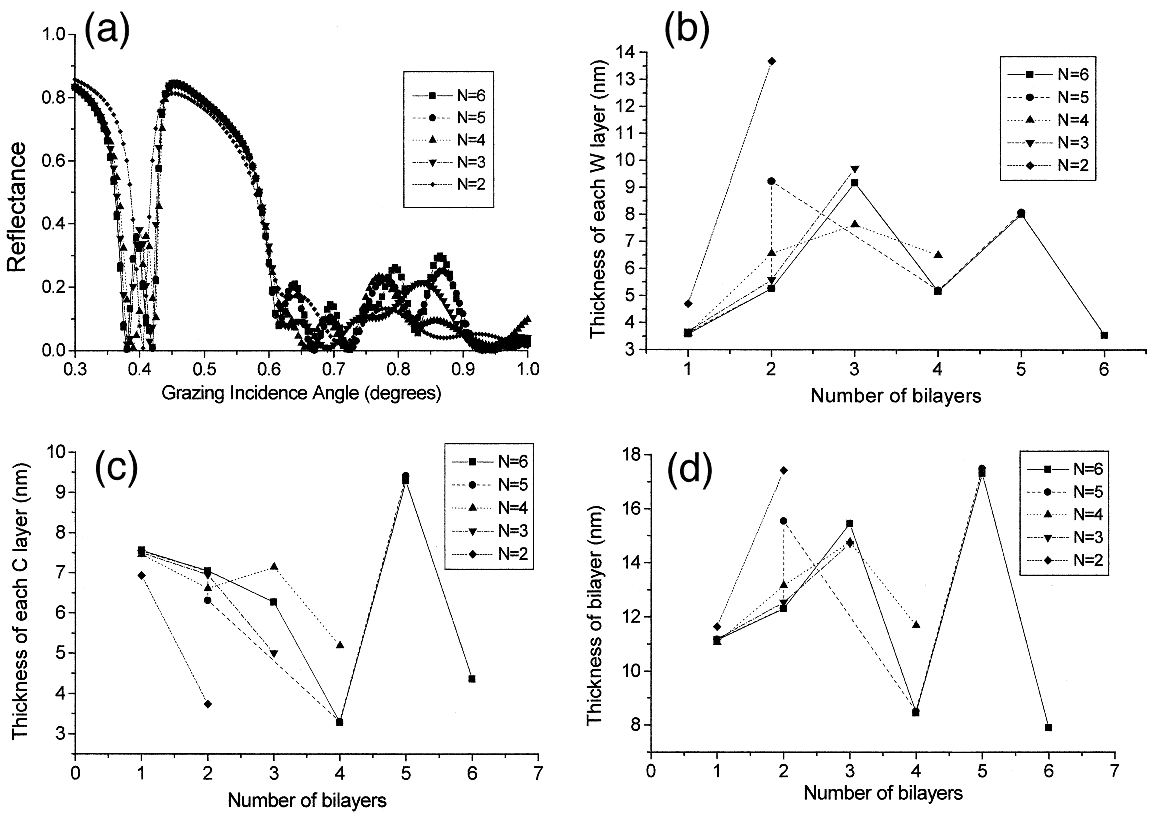

Fig. 1. (a) Calculated optimum reflectivities versus grazing incidence angle for different number of bilayers in depth-graded multilayer films, assuming 0.3 nm interfacial roughness. The shapes of the reflectivity curves are basically independent of the number, N, of bilayers in the angular interval 0.45–0.55° for $N > 2$. (b), (c) and (d) show the thicknesses of each layer (W, C and W + C); except for $N = 2$, the layer thickness variations are broadly similar for the different numbers of bilayers.

tory tradeoff was sought between increasing the reflectivity of the depth-graded multilayer and reducing its complexity by varying the total number of bilayers. A root mean square interfacial roughness of 0.3 nm was used for all the calculations.

3. Design results

3.1. High integrated reflectivity in a defined angular range

High integrated reflectivity in a defined angular range is important for multilayers to be used as condenser optics, when the collection of a large number of photons is required. Fig. 1 shows the response of a group of W/C depth-graded multilayers, with different numbers of bilayers, designed for this purpose. Each of these multilayers provides high integrated reflectivity in the angular range 0.45–0.55° for Cu Kα radiation. The highest integrated reflectivity as the number of bilayers changes requires a different distribution of bilayer thicknesses; the number of bilayers needed for high reflectivity can be very small. In this example, only 3 bilayers are needed. In Fig. 1(b)–(d) the bilayers are numbered from the top of the stack. Another feature is that the tungsten thicknesses are larger than those of carbon.

Fig. 2 shows a similar group of depth-graded W/C multilayer films designed for highest integrated reflectivity in the angular range 0.95–1.05°. Now, the shape of the reflectivity curve varies slowly and remains basically unaltered as the number of bilayers increases from 12 to 24. The thickness

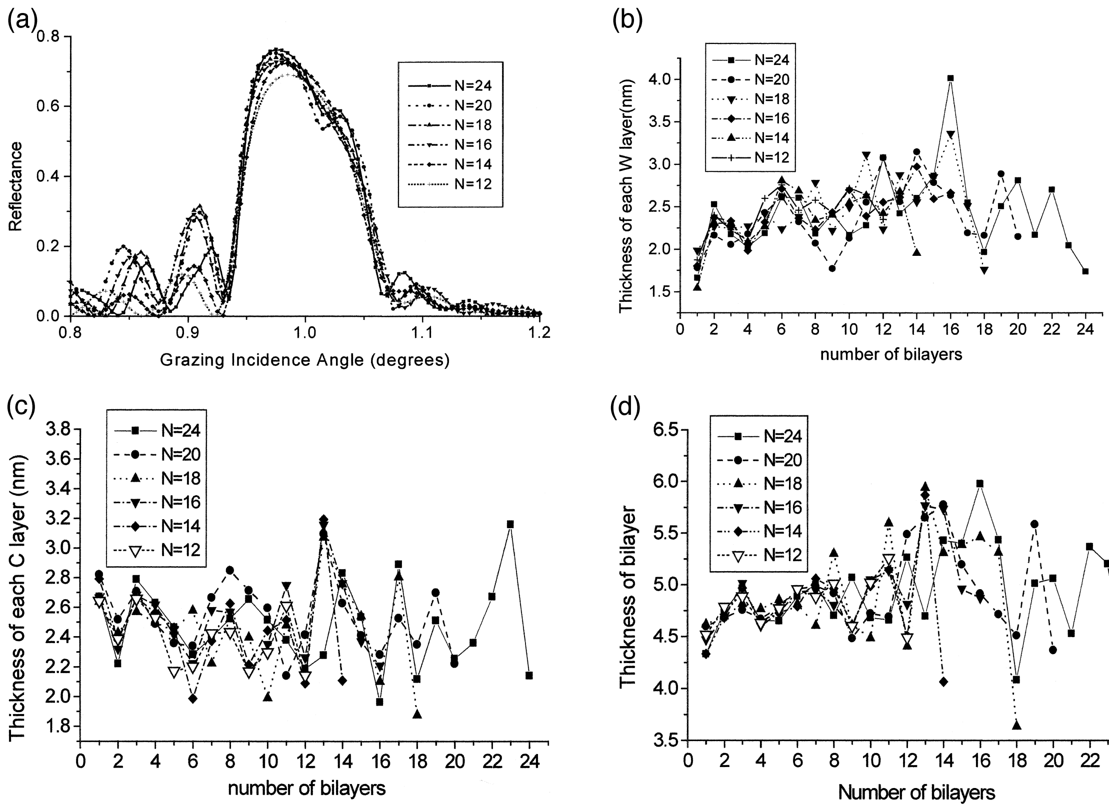

Fig. 2. As for Fig. 1, but for a different angular range. (a) The shapes of the reflectivity curves change slowly with the number of bilayers in the angular interval 0.95–1.05° when $N > 16$. Larger changes take place outside required angular interval. (b), (c) and (d) show the thicknesses of each layer (W, C and W + C); except for a few points, the layer thickness variations are approximately the same for the different numbers of bilayers.

change from layer to layer is also small and shows no obvious systematic effects. The minimum required number of bilayers is now larger, about 18 in this example. This can be explained by the variation in X-ray absorption with glancing angle, and demonstrates the importance in the design of depth-graded multilayers of determining the required minimum number of bilayers, since clearly a multilayer with few bilayers is easier to fabricate. A knowledge of the likely interfacial roughnesses in a real multilayer is also important in order to give a properly optimised design.

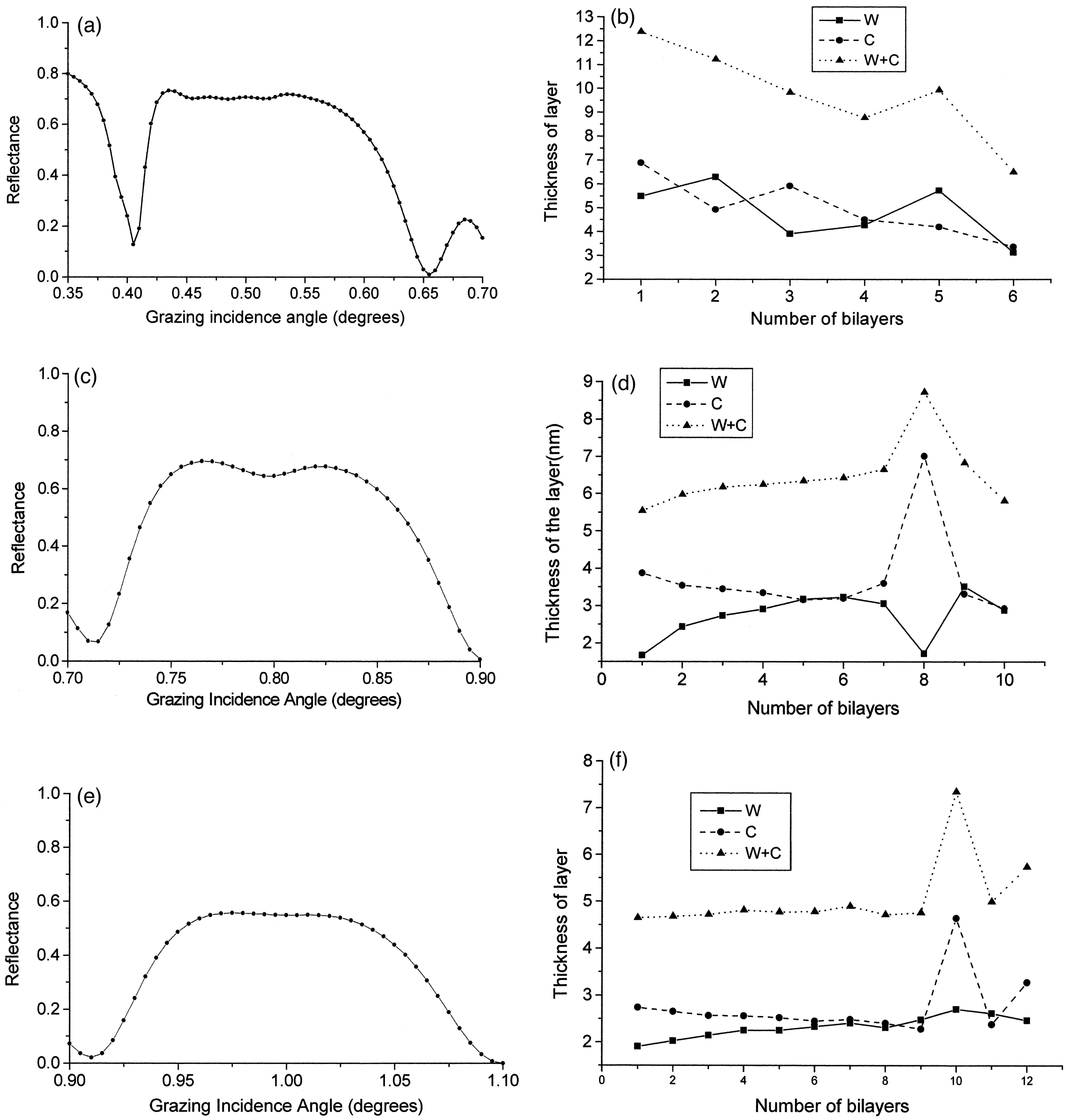

Fig. 3. (a), (c) and (e) show the optimum results in the angular ranges 0.45–0.55°, 0.75–0.84° and 0.96–1.03°, respectively. (b), (d) and (f) show the corresponding thicknesses of the layers. Although the thicknesses of the W and C layers show some quite large variations, the variation in bilayer thickness is relatively small.

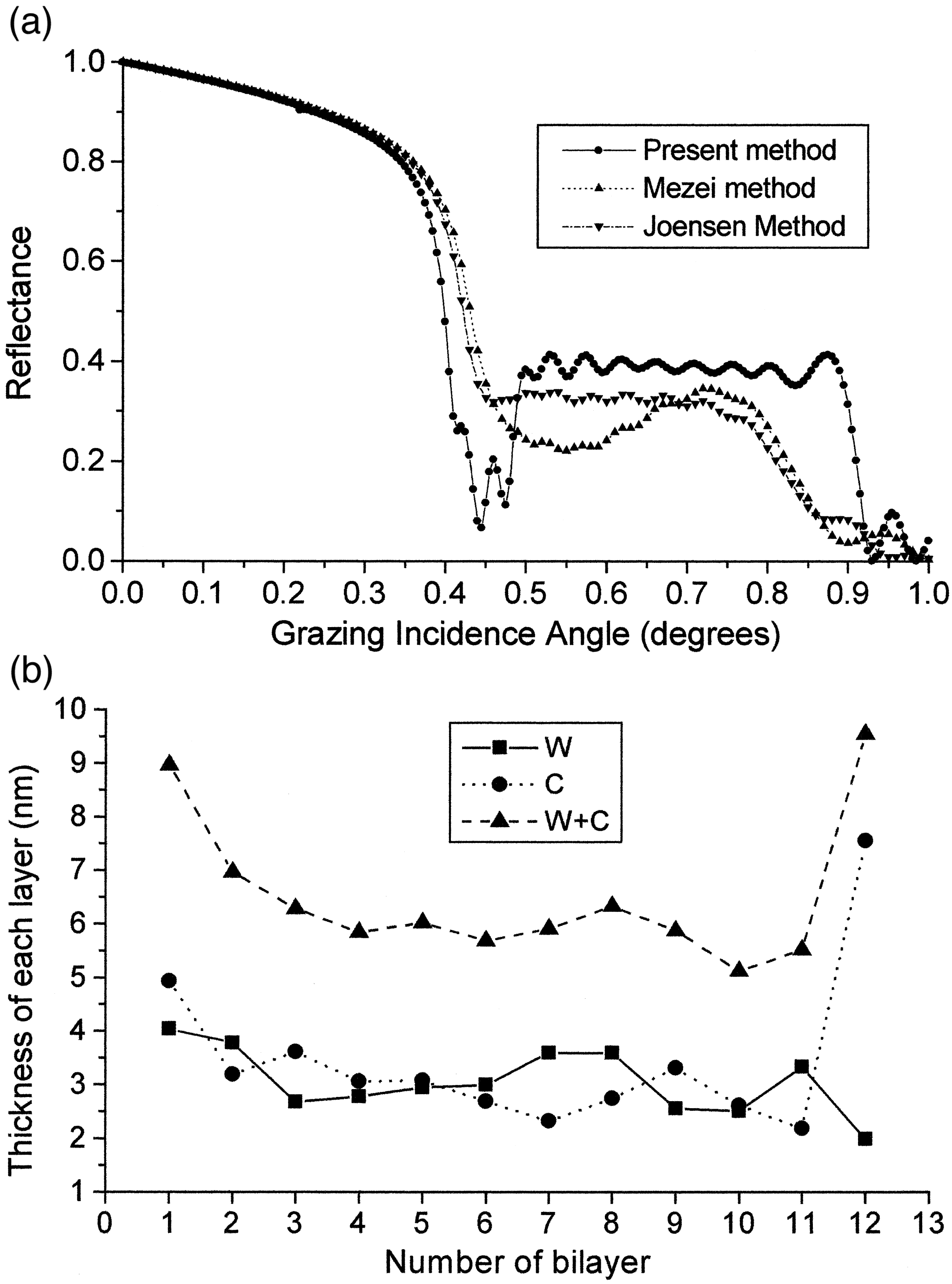

Fig. 4. (a) The calculated reflectivity responses of a depth-graded multilayers designed for a very large angular interval (0.5–0.9°) using different methods. The variations in layer and bilayer thicknesses obtained by the present method (b) are larger than for depth-graded multilayers designed for smaller angular ranges.

Table 1
Parameters of depth-graded multilayer films for $\lambda = 0.154$ nm with rms roughness 0.3 nm

	Film 1	Film 2	Film 3
Glancing angle (°)	0.5	0.795	0.995
Angular range, $\Delta\theta$ (°)	0.1	0.09	0.09
Number of bilayers	6	10	12
Average reflectivity in $\Delta\theta$	0.706 ± 0.006	0.668 ± 0.017	0.548 ± 0.008

3.2. Flat and high integrated reflectivity in a defined angular range

For some applications a flat reflectivity response, coupled with high integrated reflectivity, is desirable. For example, X-ray telescopes need to collect as much of the incident flux as possible, and in X-ray scanners the intensity of the beam during scanning (in which the incidence angle can vary) should remain as constant as possible. Fig. 3 shows three W/C depth-graded multilayer films designed to have flat and high reflectivity in different angular ranges, and their design parameters are given in Table 1. In each case, a small number of bilayers is needed, and this number changes with glancing angle.

Fig. 4 shows characteristics of a W/C depth-graded multilayer film with a wider angular range (0.5–0.9°), and its parameters are given in Table 2. The average reflectivity for Cu Kα radiation is 0.385 in this angular range, and only 12 bilayers are needed. The reflectivity curve shows some oscillations, and the thicknesses of the tungsten and carbon layers also have some variations. Fig. 4 and Table 2 also show the reflectivities of W/C multilayers with 12 bilayers and optimised parameters

(i) $d_c = 8.15$ nm and $\gamma = 0.57$ (γ is the ratio between the thickness of the absorbing layer and the bilayer period) in Mezei's model and
(ii) $a = 6.55$ nm, $b = -0.99$, $c = 0.07$ and $\gamma = 0.55$ in Joensen's model.

The results show that compared to both Joensen's and Mezei's models the present method gives more constant reflectivity (standard deviation ≈ 2.5 times lower) and a 50% higher average reflectivity over the angular range. For the calculations in Mezei's and Joensen's models the same merit function as in the present method was used. In Mezei's method there are only two parameters, d_c and γ, which need to be varied during the optimisation, which was thus fast. However, in Joensen's method there are four variable parameters, a, b, c and γ, so that the optimisation time was much longer. In the present method, it is necessary to produce several random numbers and the optimisation time is intermediate to those of Mezei's and Joensen's models.

4. Conclusion

A new method has been presented for the design of depth-graded multilayer films with high integrated reflectivity, possibly combined with a flat response, in a broad angular range. The required minimum number of bilayers can be small and depends on the grazing incidence angle. As examples of the use of the technique, several W/C depth-graded multilayer films with specified responses for Cu Kα radiation have been designed. The design results produce better multilayer performance, in terms of flatness of response and integrated reflectivity, than do existing

Table 2
Parameters of depth-graded multilayer films with very broad angular range for $\lambda = 0.154$ nm and rms roughness 0.3 nm

	Mezei's method	Joensen's method	Present method
Glancing angle (°)	0.7	0.7	0.7
Angular range, $\Delta\theta$ (°)	0.4	0.4	0.4
Number of bilayers	12	12	12
Average reflectivity in $\Delta\theta$	0.241 ± 0.043	0.266 ± 0.044	0.385 ± 0.017

methods. Although the present method does not have a gradual variation in layer thicknesses, as in previous models, this should not cause any extra difficulties in manufacture since the required thicknesses can readily be programmed as a look-up table in place of a formula.

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