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Roughness effects on the reflectance in the design of a soft X-ray multi-layer mirror

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Abstract: In the design of a multi-layer mirror at $\lambda = 1.03$ nm in soft X-ray regin, a modified method is presented, in which the effects of root-mean-square (rms) roughness of the substrate and interfaces between these films on the reflectance are considered and discussed. Then, the mathematical model for rough interfaces is given based on the scattering theory presented by D. G. Stearns. The design result shows that the substrate roughness (rms) should be smaller than 0.6 nm in order to fabricate a multi-layer mirror whose reflectance is greater than 10 %. A few super-polished fused quartz substrates with 0.5 nm (rms) roughness are chosen in coating experiments. The measured reflectance is about 10 % at $\lambda = 1.03$ nm, which is consistent with the result acquired by the modified design method. The multi-layer mirror has been applied in a X-ray spectrograph for diagnosis of inertial confinement fusion (ICF).

Key words: roughness; reflectance; multi-layer mirror

软 X 射线多层膜设计中表面粗糙度对反射率的影响

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摘要:给出了一种改进的软 X 射线波段的多层膜设计方法。在设计过程中,考虑了反射镜基底和各膜层之间的均方(RMS)粗糙度对反射率的影响;在 Stearns 提出的散射理论的基础上给出了粗糙界面的数学模型。文中以波长为 $\lambda = 1.03$ nm的软 X 射线为例进行设计,设计结果表明:要使波长为 $\lambda = 1.03$ nm 的多层膜的反射率大于 10 %,反射镜基底的均方粗糙度不应超过 0.6 nm。实验中选择几块表面粗糙度为 0.5 nm(RMS)的熔石英平面镜作为基底来制作适用于该波长的、层对数超过 70 的多层膜。然后在的入射角下测量反射率,测得的值为 10 %,这与采用本设计方法得到的计算结果一致。该反射镜作为 X 射线谱仪的分光元件被应用于惯性约束聚变(ICF)的过程诊断中。

关　键　词:粗糙度;反射率;多层膜
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1 Introduction

Multi-layer reflecting mirrors have many applications in X-ray region, for example, inertia confinement fusion (ICF), astronomy and biological microscopy[1-4]. In the longer wavelength region of soft X-ray ($\lambda > 10$ nm), high peak reflectance of Mo/Si multi-layer mirrors have been obtained at several wavelengths, for instance, the peak reflectance at $\lambda = 13.4$ nm reachs 66 %[5]. But in the shorter wavelength region of soft X-ray ($\lambda < 10$ nm), the fabrication of multi-layer mirrors with high reflectance is still in research and development, and the measured reflectance is much lower than that of the theoretically designed. The main reason is that there are rough surfaces, including substrate and interfaces between the films. In the shorter wavelength region of soft X-ray, the value of roughness has a greater effect on reflectance than that in the longer wavelength region. So in order to fabricate multi-layer mirrors with high reflectance in this region, it is essential to consider the effect of roughness.

In the processes of designing and fabricating multi-layer mirrors, the first thing is to select the best matching material pairs which can form smooth and compositionally abrupt interfaces, and have a high optical contrast and minimal absorption. And then the roughness of the substrate and interfaces is assummed to be zero. According to the iterative or matrix method of the multi-layer film theory, calculations are done to gain muti-layer structure parameters (including the period number, the thickness of each period and the ratio of material pairs). Although the theoretical reflectance of the design method is very high, the measured reflectance after deposition is very low. The reason is that flaws of the substrate and interfaces are not considered, so the design cannot give an exact anticipation of reflectance. In order to overcome the shortcoming, a modified design method is proposed in which the roughness of the substrate and interfaces is considered in designing of a multi-layer mirror. Because of considering the roughness, appropriate scattering theory to describe non-ideal interfaces is needed. In our project, D. Stearns's scattering theory is used because it is suitnble for the region of the shorter wavelength in soft X-ray. A multi-layer mirror at the wavelength of 1.03 nm in soft X-ray region is deposited in our project, whose peak reflectance is required above 10 %. Applying the modified method, the calculated reflectance is basically consistent with the measured reflectance.

2 Theory

2.1 Designing foundation of multi-layer mirrors

The recursive formula from the theory of optical thin film is used in designing multi-layer mirrors[6]. The optical constants of B. L. Henke are adopted to be the data in this paper[7]. In general, the interference of thin film is the interference of several ray beams. Assuming that r_1 and r_2 are the reflectance coefficients of two interfaces in a single film, respectively, the total complex reflectance of the single film system can be expressed by the following equation

$$r_f = \frac{r_1 + r_2 \exp(2i\delta)}{1 + r_1 r_2 \exp(2i\delta)}, \tag{1}$$

where $\delta = 2\pi nd\cos\alpha/\lambda$. Equation (1) is effective to any-layer thin film and can also be adapted to multi-layer mirrors. The total reflectance of a multi-layer films with N layers can be obtained through using equation (1) repeatedly.

At $\lambda = 1.03$ nm in soft X-ray region, the best pair of material is Pt/Si, because it has a smooth interface and a high optical contrast. Assuming that the roughness of the substrate and interfaces between the films is equal to zero, the reflectance is calculated according to equation (1) and the results are listed in Table 1.

Tab. 1 The designed results of Pt/ Si multi-layer with an ideal interface

Material	Wavelength	Incidence angle	Period	d_{Pt} (nm)	d_{si} (nm)	r
Pt/ Si	1.03 nm	80.7°	70	1.45	1.85 nm	40 %

Table 1 shows the assumed ideal interface results. From Table 1 we know that the peak reflectance is 40 %. But since there is a flaw on the substrate and interfaces between the films, the results cannot give the exact anticipation value of an actual mutilayer mirror with roughness. In our following design, the effect of roughness based on the scattering theory presented by Stearns is considered.

2.2 Scattering theory about non-ideal interface

In the scattering theory of D. Stearns[8], the interface profile function $p(z)$ for describing a non-ideal interface is used. The $p(z)$ is defined as the normalized average value of the dielectric function along z direction.

$$p(z) = \frac{\iint \varepsilon(x)\,\mathrm{d}x\,\mathrm{d}y}{(\varepsilon_i - \varepsilon_j)\iint \mathrm{d}x\,\mathrm{d}y}, \qquad (2)$$

where $\varepsilon(x) = \begin{cases} \varepsilon_i & z \to +\infty \\ \varepsilon_j & z \to -\infty \end{cases}$

According to Stearns's scattering theory, if r and $\tilde{r}$ are the Fresnel reflectance coefficients of an ideal and a non ideal interface, respectively, then the modified Fresnel formula can be expressed by

$$\tilde{r} = r\,\tilde{w}(s), \qquad (3)$$

where $w(z) = dp(z)/d(z)$. The Fourier transform of $w(z)$ is $w(s)$, where $s = 4\pi\cos\alpha/\lambda$.

3 Modified designing method and result

The modified design method is that the effect of the roughness on the reflectance is considered in designing multi-layer mirrors at $\lambda = 1.03$ nm. When recursive formula (1) is applied, r_2 is replaced by coefficient r in formula (3). So the effect of the roughness on the reflectance is expressed in the form of interface profile function obtained from Stearns results.

The impact of the roughness of the substrate on the interface between films may be copied in the coating process layer by layer or amplified/ reduced. The value of the interface roughness is around the value of the substrate roughness, so the value of the interface roughness is assumed to be the same as the substrate roughness in the Pt/ Si multi-layer.

For the sake of realizing the aim of peak reflectance above 10 % at $\lambda = 1.03$ nm, the modified method is used in the calculation process of a Pt/ Si multi-later mirror. For different roughness value, formula (3) is substituted into formula (1) to do recursive calculation and then the reflectance is obtained. In accordance with the calculation results, R-σ curves are plotted in Fig. 1 through Fig. 4. From the figures the minimal value of the roughness satisfying the design requirement can be found. In calculations, a mathematical model to describe the nonideal interface is needed. We describe the interfaces using four interface profile functions introduced by Stearns' scattering theory. The four interface profile functions of $p(z)$, and their Fourier transforms, $w(s)$, of their responding derivatives are listed in Table 2.

When $\lambda = 1.03$ nm and the incidence angle is 80.7°, calculations were made based on the mathematical models in Table 2, using equation (1) and Fresnel's modified fomula (3). The R-σ curves figures 1 through 4 show the calculated results.

The horizontal axes in the figures show the roughness and the vertical axes show the reflectance. From the curves above, we can conclude that the average roughness value should not exceed 0.6 nm in order to realize the aim in which the reflectance is higher than 10 %.

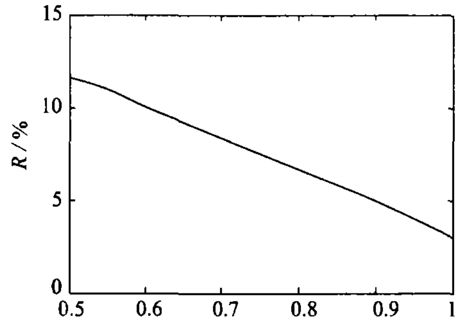

Fig. 1　R-σ curve with error function

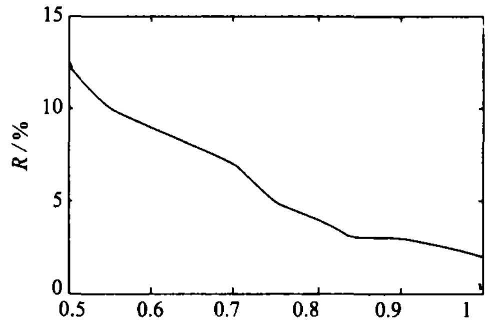

Fig. 3　R-σ curve with exponential function

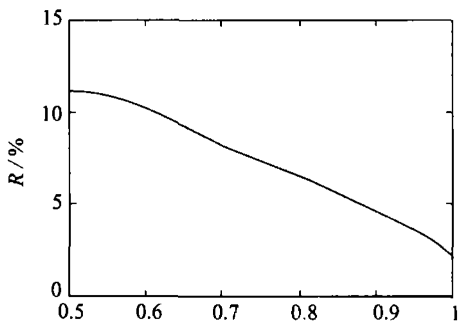

Fig. 2　R-σ curve with r linear function

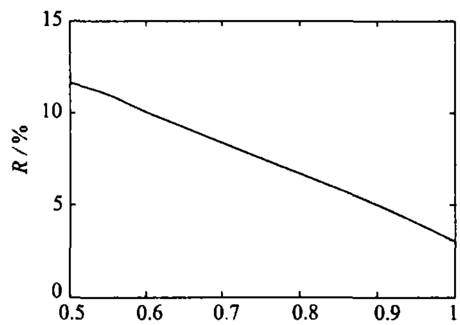

Fig. 4　R-σ curve with sinusoidal function

Tab. 2　Several useful profiles and functions p(z) **and** w(s)

Function types	$p(z)$	$w(s)$
Error function	$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{z} e^{-t^2/2\sigma^2}dt$	$e^{-\sigma^2 s^2/2}$
Linear	$\begin{cases} 0 & z < -a\sigma \\ \frac{1}{2}+\frac{1}{2}\sin(\frac{\pi z}{2a\sigma}) & \lvert z\rvert < a\sigma \\ 1 & z > a\sigma \end{cases}$	$\frac{\sin(\sqrt{3}\sigma)}{\sqrt{3}\sigma s}$
Exponential	$\begin{cases} \frac{1}{2}e^{2z/\sigma} & z \le 0 \\ 1-\frac{1}{2}e^{2z/\sigma} & z > 0 \end{cases}$	$\frac{1}{1+s^2\sigma^2/2}$
Sinusoidal	$\begin{cases} 0 & z < -\sqrt{3}\sigma \\ 1/2 + z/2\sqrt{3}\sigma & \lvert z\rvert < \sqrt{3}\sigma \\ 1 & z > \sqrt{3}\sigma \end{cases}$	$\frac{\pi}{4}\left(\frac{\sin(a\sigma-\pi/2)}{a\sigma-\pi/2}+\frac{\sin(a\sigma+\pi/2)}{a\sigma+\pi/2}\right)$

4　Xperimental results and conclusions

The results above show that the substrate roughness should be smaller than 0. 6 nm in order to fabricate a multi-layer mirror whose reflectance is greater than 10 %. So we use fused quartz as the substrate material. The plane of the material is polished to 0. 5 nm (rms) for its roughness. Pt/ Si multi-layer films are deposited on the polished plane of the substrate.

The deposited multi-layer mirror was measured with synchronization radiation equipment at Beijing Institute of High Energy. The measured results are shown in Figure 5.

Fig. 5 shows that the peak reflectance is about 10 % at $\lambda = 1.03$ nm. The result means that the

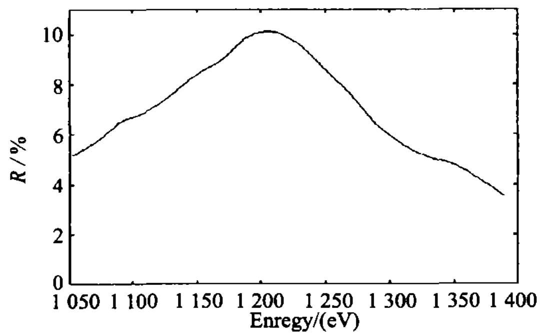

Fig. 5 Measurement curve of reflectance

design result of the modified method is consistent with the measurement result. In order to explain the advantages of the modified method, we have deposited a W/ Si multi-layer mirror with a 1 nm substrate using the same method and measured its reflectance with the same synchronization radiation equipment. Although the theoretical reflectance is 38 %, the measured peak reflectance is only 1. 7 %. So it is clear that the reflectance value of the multi-layer mirror designed by the modified method is consistent with the measured value.

The following conclusions can be deduced. (1) In order to fabricate a multilayer mirror with high reflectance in soft X-ray region, the roughness should be smaller than a specified value; (2) The modified method is feasible to seek for rms roughness of the prescriptive value; (3) The method can provide a right anticipation before deposition and give a valuable reference for practical deposition.

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