Influence of interface roughness on reflectivity of tungsten/boron-carbide multilayers with variable bi-layer number by X-ray reflection and diffuse scattering

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Received November 5, 2008

Influence of interface roughness on the reflectivity of Tungsten/boron-carbide (W/B_4C) multilayers varying with bi-layer number, N, is investigated. For W/B_4C multilayers with the same design period thickness of 2.5 nm, a real-structure model is used to calculate the variation of reflectivities with N = 50, 100, 150, and 200, respectively. Then, these multilayers are fabricated by a direct current (DC) magnetron sputtering system. Their reflectivity and scattering intensity are measured by an X-ray diffractometer (XRD) working at Cu Kα line. The X-ray reflectivity measurement indicates that the reflectivity is a function of its bi-layer number. The X-ray scattering measured results show that the interface roughness of W/B_4C multilayers increases slightly from layer to layer during multilayer growing. The variation of the reflectivity and interface roughness with bi-layer number is accurately explained by the presented real-structure model.

OCIS codes: 310.0310, 220.0220, 230.0230, 340.0340.
doi: 10.3788/COL20090708.0738.

Tungsten/boron-carbide (W/B_4C) material combination has already been identified as a promising X-ray multilayer structure for ultra-thin period[1−4] and developed for many applications[5,6] in hard X-ray region. For example, for the multilayer mirror working at Cu $K\alpha$ line, wavelength $\lambda = 0.154$ nm, the ultra-thin period D, and great bi-layer number N, are required to obtain enough effective reflectivity. Because the layer thickness is ultra-thin, the imperfection in multilayer structure will significantly reduce its performance. Considering the imperfection in multilayer, the reflectivity of a multilayer can be calculated by the Nevot-Croce model[6−8]:

$$\mathrm{M}_j = \exp\left[-\frac{1}{2}\left[\frac{4\pi\sigma}{\lambda}\right]^2 \sin\theta_{i-1}\sin\theta_i\right], \quad (1)$$

$$n_0\cos\theta_0 = n_i\cos\theta_i, \quad (2)$$

$$R_{\mathrm{real}} = M_i R_{\mathrm{ideal}}, \quad (3)$$

where n_0 is the optical constant of incident medium, σ is the root mean square (RMS) value of the effective roughness, n_i is the optical constant of the ith layer, and θ_i is the grazing incidence angle in the ith layer, R_{real} and R_{ideal} are the amplitude reflectivities of the real multilayer and the ideal one, respectively. The structures of the real and ideal multilayer are shown in Figs. 1(a) and (b), respectively.

In this model, there are three parameters: layer thicknesses of each material, d_1 and d_2 ($D = d_1 + d_2$), and the interfacial roughness factor σ, which is a constant from layer to layer. It is accurate enough for multilayers with not too many bi-layer pairs. However, for multilayer with large number of bi-layer pairs, some investigations showed that the interfacial roughness of a multilayer would vary[9−11] and the reflectivity of such a multilayer could be accurately calculated by a so-called real-structure model, as shown in Fig. 1(c). In this mode, the statistical roughness growth from layer to layer is accepted as the law of the structure growth[9]:

$$\sigma_i = \sqrt{\sigma_0^2 + h(x_i - x_0)}, \quad (4)$$

where σ_0 is the roughness of the substrate, σ_i is the roughness of the ith interface, and x_0 and x_i are the mean value of the coordinate of the substrate and the ith interface along the direction perpendicular to the layers, respectively. The parameter h is a constant, which defines the rate of the roughness from layer to layer. The units of the parameters, h, σ_0, σ_i, x_0, and x_i, are nanometer. Substitute Eq. (4) into Eq. (1)

$$\mathrm{M}_j = \exp\left[-\frac{1}{2}\left[\frac{4\pi\sigma_i}{\lambda}\right]^2 \sin\theta_{i-1}\sin\theta_i\right]. \quad (5)$$

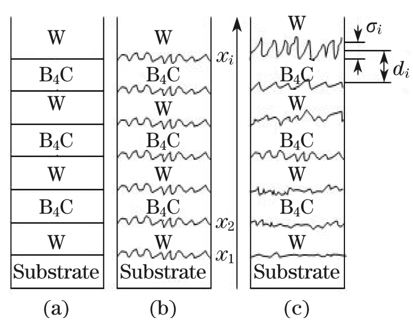

Fig. 1. Structure of (a) an ideal-structure multilayer, σ=0, (b) practical multilayer, σ being constant, and (c) the real-structure multilayer, σ being variable from layer to layer.

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The reflectivity of a real-structure model multilayer should be simulated by Eqs. (2), (3), and (5). In Fig. 2, the peak reflectivity (PR) curves of W/B_4C multilayer mirrors with variable bi-layer pairs are calculated respectively based on the three models up-introduced at Cu Kα line. The calculation results present that PRs of multilayers are functions of their bi-layer pairs. For ideal (solid-line) and Nevot-Croce model (dot-line) multilayer, PRs of multilayer increase with the bi-layer pairs rising and tend to saturate with bi-layer pairs of more than 100, because of the absorption of layer materials. For the real-structure model (dash-line) multilayer, its PR increases firstly and gets to the maximum value (N = 100), and then decreases as its bi-layer pairs enhance.

In order to verify the calculation shown in Fig. 2, a series of W/B_4C multilayers with bi-layer number N = 50, 100, 150, and 200, respectively, were fabricated by DC magnetron sputtering on super-polished silicon substrates. All the substrates were cut from the same super-polished Si wafer (6 inch in diameter) into the size of 30×40 (mm), so the surface roughnesses of these substrates could be considered as the same value. All the substrates were cleaned by acetone and ethanol before coating. The base pressure was 5.7×10^{-5} Pa before depositing. The sputtering gas was argon (Ar) (with purity of 99.999%), at the constant pressure of 0.13 Pa during the deposition. After deposition, the reflectivities and periods of those W/B_4C multilayers were measured by a grazing-incident X-ray Diffracometer (XRD) working at Cu $K\alpha$ line (D1 system, Bede Inc., UK). The measured results are shown in Fig. 3. The peak reflectivity of W/B_4C multilayer, with bi-layer number $N = 50$, is only 57%. The multilayers with bi-layer number $N = 100$ and 150, have the same peak reflectivity of 69%, which is the highest reflectivity. For the multilayer with the largest bi-layer number $N = 200$, the peak reflectivity is 65%, lower than that with bi-layer number $N = 100$. In Fig. 3, the curves of reflectivity are not superposition, which results from the little discrepancy of period thickness between designed and fabricated multilayers. The discrepancy will not influence the comparison of peak reflectivity because the maximum periodic discrepance of those multilayers is 0.033 nm, which is 1.32% of the expecting period of 2.5 nm.

The measured reflectivities shown in Fig. 3 do not increase when the bi-layer number N is larger than 100, which indicates that interface roughness of multilayer varies during the layer growing. So the scattering intensity of these multilayers was measured to characterize their interfacial roughness[12,13]. The rocking scan curves of the first order Bragg peak were measured by XRD using θ-scan model. The rocking scan curves are shown in Fig. 4. It can be seen clearly that the scattering intensity of W/B_4C multilayers increases with the bi-layer number. Calculated results shown in Fig. 2 exhibit that the X-ray beam could penetrate about 100 W/B_4C bi-layer pairs because of the absorption of the layer materials. For W/B_4C multilayers with bi-layer number of N = 100, 150, and 200, the number of interface contributing to the scattering intensity will be the same of $2N$ = 200. And the X-ray scattering measurements show that the interfacial roughness of W/B_4C multilayers increases from layer to layer in their growth direction. For W/B_4C multilayer with bi-layer number of $N = 50$, the interface contributing to scattering intensity is only $2N = 100$, lower than 200. So, the scattering intensity is weaker than that of multilayers with larger layer number.

The real-structure model (expressed in Eq. (5)) could explain the evolvement of the PR of multilayer with bi-layer number N. Figure 5 shows the comparison between the measured peak reflectivities (Fig. 3) and the calculated results using Eq. (5) (Fig. 2(c)). It can be seen that the theoretical curve agrees with the measured data, which indicates that the interfacial roughness of W/B_4C multilayer increases slightly from layer to layer in its growth direction.

In conclusion, both the reflectivity and scattering measurements show that the interfacial roughness of W/B_4C multilayer increases slightly from layer to layer in layer growing direction, and the reflectivity of multilayer is

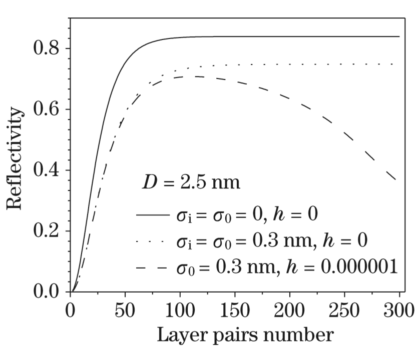

Fig. 2. Calculated PR curves of the W/B_4C multilayers, D = 2.5 nm, based on different multilayer structure models for ideal model (solid-line), Nevot-Croce model (dot-line), and real-structure model (dash-line), respectively.

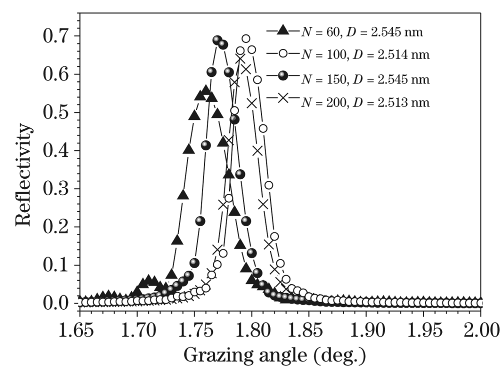

Fig. 3. Measured reflectivities of W/B_4C multilayers with variable bi-layer pairs.

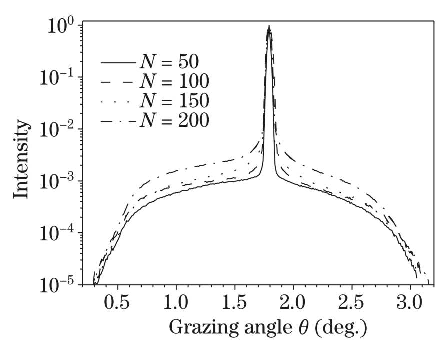

Fig. 4. Measured rocking scan curves of the W/B_4C multilayers with different bi-layer pairs at wavelength $\lambda = 0.154$ nm.

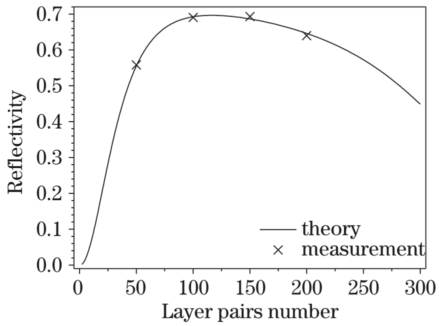

Fig. 5. Measured PRs of W/B_4C multilayers and the theoretical curve based on the real-structure model.

a function of its bi-layer number. In our investigation, the reflectivity of the W/B_4C multilayer increases with the bi-layer number N firstly, and reaches the maximum when the bi-layer number is 100. However, when the bi-layer number is larger than 150, the reflectivity of multilayer decreases. The variation of the reflectivity with bi-layer number could be accurately explained by the real-structure model expressed in this letter.

This work was supported by the National Natural Science Foundation of China (Nos. 10435050, 10675091, and 10675092), the National "863" Project of China (No. 2006AA12Z139), the Science and Technology Commission of Shanghai Municipality (No. 07DZ22302), and the Program for Young Excellent Talents in Tongji University.

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