XAFS Study on the Microstructure of Mo/Si Multilayers

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XAFS Study on the Microstructure of Mo/Si Multilayers

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Abstract X-ray absorption fine structure(XAFS) was used to investigate the structure of Mo/Si multilayers from 20Å to 3000Å period value. The XAFS results show the structural disorder of Mo atom neighbor environment is significantly increased as the thickness of Mo layer is thinner. For 20Å and 50Å period Mo/Si multilayers, the polycrystalline Mo layer vanish, the first neighbor coordination of Mo atom is mainly surrounded by Si atoms, the intended small period structure were drastically destroyed by interdiffusion. The mixed layer is amorphous $MoSi_2$. XAFS results confirm that there is no clear period structure in very small period Mo/Si multilayer.

1. Introduction

In recent years, there has been accelerating interest in period Mo/Si multilayers used as reflective and dispersive elememts at soft X-ray waveband. It was reported that the reflectivities of Mo/Si mirrors, which were fabricated for the wavelength region of 125~250Å[1], can reach 50%. The structure studies of Mo/Si multilayer revealed that there were clear interfaces between Si and Mo layer, a-Si and polycrystalline Mo in these samples[1, 2]. However, the internal microstructure of the individual Mo layers and Mo/Si interfaces are not known clearly now. In this short report, Our aims were to study the local structural change of Mo atomic neighbor environment of Mo/Si multilayers with the period decrease by XAFS.

2. Experimental

Mo/Si multilayers with periods of 20Å, 50Å and 200Å were deposited on cleaned glass substrates with a magnetron sputtering apparatus. The Ar sputtering pressure was 1.00Pa. Deposited rates of Si and Mo were 32Å/min and 27Å/min, respectively. The thickness ratio of Mo and Si is 1:2 in all Mo/Si multilayers. Mo film with thickness of 3000Å was also fabricated with deposition. The Mo K-edge XAFS spectra of the peeled samples were measured on the beam line of 4W1B of Beijing Synchrotron Radiation Facility. The electron beam energy is 2.2GeV and maximumstored current is 50mA. Data were collected with a fixed exit monochromator using two flat Si(111) crystals. Data were collected in transmission mode using ion chamber fill with Ar gas at room temperature.

3. Results and Discussion

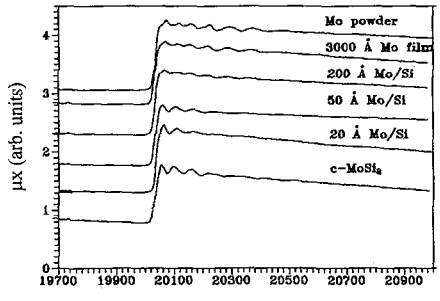

Fig.1 Mo K-edge Absorption Spectra of Mo/Si Multilayers

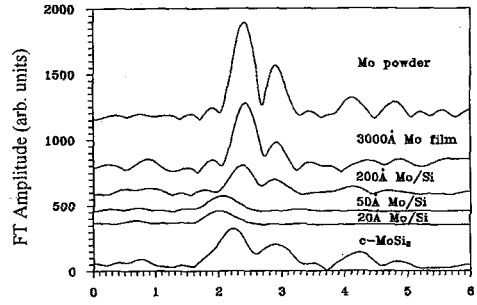

Fig.2 The RDF of Mo Atom of Mo-Si Multilayers

The Mo K-edge absorption spectra of Mo/Si multilayers, crystalline Mo powder and $MoSi_2$ film are shown in Fig. 1. It can be found that intensity and frequency of the oscillatory signal decreased for small period Mo/Si multilayers. In the 400eV above the Mo K absorption edge, there are six oscillation peaks for Mo powder and 3000Å Mo film, only two peaks for 50Å and 20Å period Mo/Si multilayers. The absorption spectra of 20Å and 50Å Mo/Si multilayers are evidently different from that of 3000Å Mo film. Otherwise, they are similar to that of $MoSi_2$ in the 0 to 200eV region above Mo absorption edge except the amplitude of modulation is a little lower.

Fig. 2 shows the radial distribution functions (RDF) of samples, which were obtained from fast Fourier transformation of their $\chi(k)k^3$. There are two stronger coordination peaks at 2.40Å and 2.90Å in the RDF of Mo powder, it may contribute to the first shell R=2.72Å, N=8, and the second shell R=3.14Å, N=6 respectively. In the RDF of $MoSi_2$ film, the first main peak is that Mo is coordinated by ten Si atoms, $R_{Mo\text{-}Si}$=2.62Å; the second stronger peak is that Mo is coordinated by four Mo atoms, $R_{Mo\text{-}Mo}$=3.20Å. Compared with 3000Å Mo film, the peak amplitude of the first and second Mo coordination shell decrease drastically for the 200Å period Mo/Si multilayer, but their R values are equal. It suggests that the Mo local structure of Mo/Si multilayer with 200Å period keeps the main characteristic of metallic Mo, their differences are structural disorder. The RDF shapes of both 20Å and 50Å period Mo/Si multilayers are the same, which are evidently different from that of 200Å Mo/Si multilayer, only one weak amplitude peak appears at R=2.00Å. It indicates that Mo is complete amorphicity for the 20Å and 50Å period Mo/Si multilayers because peaks of farther distant neighbors are absent.

For systems having a high degree of crystalline order or small disorder as the 3000Å Mo film, the pair distribution function of neighbor atoms around the absorbing atom can be assumed as a symmetric Gaussian function:

$$g(R) = (2\pi\sigma^2)^{-1/2}\exp[-(R-R_0)^2/2\sigma^2] \quad (1)$$

The expression of XAFS interference function as:

$$\chi(k) = \Sigma_j N_j F_j(k) S_0^2(k)/kR_j^2 \cdot \exp(-2R/\lambda(k))\exp(-2k^2\sigma_j^2) \cdot \sin[2kR_j + \delta(k)] \quad (2)$$

For disordered systems, the Gaussian pair distribution function is unvalid to express the neighbor atoms distribution from central atom. The asymmetric distribution function of disordered Mo/Si multilayers with 20Å to 50Å period is designed as:

$$\begin{aligned} g(R)asym &= (1/\sigma_S)\exp[-(R-R_0)/\sigma_S] && R \geq R_0 \\ &= 0 && R < R_0 \end{aligned} \quad (3)$$

$$\chi(k)_1 = N_1 F(k) S_0^2(k)/kR_0^2 \cdot 1/(1+4k^2\sigma_S^2)^{1/2} \cdot \exp(-2R/\lambda(k))\exp(-2k^2\sigma_t^2) \cdot \sin[2kR + \delta(k) + \arctg 2k\sigma_S] \quad (4)$$

$\chi(k)_1$ is the XAFS function for the first coordination shell. σ_S is the root mean square displacement of structural disorder, σ_t is the thermal disorder, R_0 is the distance of central atom to the closest packing atom. The differences between equation (2) and (4) are a reduced factor $1/(1+4k^2\sigma_S^2)^{1/2}$ in amplitude and a term $\arctg(2k\sigma_S)$ in phase shift.

Table 1. The Structural Parameters of Mo/Si Multilayers

			first neighbor coordination shell								
sample		pair	R(Å)	σ_t(Å)	σ_S(Å)	N	pair	R(Å)	σ_t(Å)	σ_S(Å)	N
3000Å Mo film		Mo-Mo	2.73	0.065	~0	8.0±0.5					
200Å	Mo/Si	Mo-Mo	2.71	0.091	~0	6.2±0.5	Mo-Si	2.60	0.065	~0	1.2±0.3
50Å	Mo/Si	Mo-Si	2.61	0.071	0.080	5.8±0.5	Mo-Mo	2.70	0.072	0.11	1.4±0.3
20Å	Mo/Si	Mo-Si	2.60	0.073	0.085	6.0±0.5	Mo-Mo	2.69	0.075	0.12	1.5±0.3

The results in table 1 show that the disorder factor σ($\sigma = \sigma_t + \sigma_s$) of Mo atoms increase while the thickness of Mo layer is thinner. Though the main peak R value is contracted 0.4Å and peak magnitude intensity is many time lower for 20Å and 50Å period Mo/Si multilayers comparing with 3000Å Mo film, we can obtained reasonable structural parameters by assuming the pair distribution function as $g(R)_{asym}$. For small period Mo/Si multilayers, the σ_s is bigger than the σ_t and the first coordination shell of Mo atom is mainly coordinated by Si atom. It means the interdiffusing region of both Mo and Si layer is thicker than 16.7Å the intended thickness of Mo layer, and the structure of mixed layers is considered as amorphous $MoSi_2$. There are not polycrystalline Mo layer in small period Mo/Si multilayers. Fabricating with magnetron sputtering apparatus, it is difficult to obtain a clear interface between Mo and Si layer while the individual layer is thin to about 15Å.

Acknowledgments

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