Transmission characteristics of multilayer structure in the soft x-ray spectral region and its application to the design of quarter-wave plates at 13 and 4.4 nm

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The increasing usage of soft x-ray radiations due to the development of synchrotron radiation source and others demands varied optical manipulation in the soft x-ray spectral region. The phase manipulation is important because this leads to the control of the polarization state of a soft x-ray radiation. A new criterion for selecting material pairs for the maximum phase difference between the *s* and *p* polarization through a multilayer (ML) structure was proposed and tested theoretically. Transmission characteristics of ideal ML structures in the soft x-ray spectral region have been studied by simulation. The results have been applied to optimize ML structures for quarter-wave plates at 4.4 and 13 nm. It was found that Rh/Si and Co/K MLs are good candidates for quarter-wave plates at 13 and 4.4 nm, respectively.
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I. INTRODUCTION

The increasing usage of circularly polarized x-ray radiation in scientific fields, one of which is the study of magnetic circular dichroism,[1–4] has demanded the phase control of x-ray radiation. Such a demand has recently increased research for the development of linear polarizers, phase shifters and quarter-wave plates in the soft x-ray spectral region. The possibility of a multilayer (ML) structure as a quarter-wave plate was studied by Kortright and Underwood.[5] They showed that a Mo/Si ML having 20 bilayers can produce enough phase difference for a quarter-wave plate at 13 nm. Kortright *et al.*[6] fabricated a Mo/Si ML with 20 bilayers and obtained a maximum phase retardation at 13 nm of 49° and a transmittance ratio of 0.66 between the *s*- and *p*-polarized light at the maximum phase difference. Nomura *et al.*[7] also fabricated a Mo/Si ML with 81 bilayers using a magnetron sputtering system and obtained a phase retardation of 90° and a transmittance ratio of 1.66 between the *s*- and *p*-polarized light with a throughput of around 10%. Di Fonzo[8] suggested optimized structures for transmission ML as a quarter-wave plate in the soft x-ray region and reported the transmission characteristics of a Cr/C ML with 100 bilayers near the carbon K edge.[9] In this work, we have done detailed studies on the phase properties of transmitted soft x-ray radiation through a ML: the dependence of the phase on the material combination, the incident angle of light, the thickness ratio of the constituent materials, the number of bilayers, and the imperfections at the interfaces. Previously it was not clear how to choose materials for maximizing the phase difference between the *s* and *p* polarization but the same criterion used for high-reflectivity ML reflectors has been used. A new criterion of selecting materials for the maximum phase difference was proposed and tested. The results of these studies have led us to propose better ML candidates as transmission quarter-wave plates at 13 and 4.4 nm.

II. MODEL OF CALCULATION

Figure 1 shows the schematic diagram of an ideal ML structure. In each layer, a forward-propagating electric field (E_j) and a backward-propagating field (E_j^R) with the corresponding magnetic fields are considered. At each interface these fields should satisfy the boundary conditions imposed by Maxwell's equations. In this way, the fields in a layer are connected in other layers, automatically taking multiple reflections into account.

Following the recursive method,[10,11] whose results have been in good agreement with experimental results within experimental error and extensively used,[12,13] one can get the following recursive relationship for transmission:

$$T_j^{s,p} \equiv a_j a_{2N+1} \frac{E_{2N+1}^{s,p}}{E_j^{s,p}} = a_j^2 \frac{1+F_{j,j+1}^{s,p}}{1+F_{j,j+1}^{s,p} R_{j+1}^{s,p}} T_{j+1}^{s,p}, \tag{1}$$

where $R_j^{s,p} \equiv a_j^2 E_j^{R,s,p}/E_j^{s,p}$, $a_j = \exp(-ig_j \pi d_j/\lambda)$, $g_j = n_j \sin\theta_j$ with $i=\sqrt{-1}$, and λ is the wavelength of the incident light. The input angle θ refers to the grazing angle of incidence and fields are evaluated in the middle of each layer in this study. $F_{j,j+1}^{s,p}$ is the Fresnell reflection coefficient at an interface. The subscripts s and p represent the s and p polarizations, respectively. T_j is the transmission amplitude for a ML with $(2N-j)$ layers. The successive application of Eq. (1) with the initial conditions of $R_{2N+1}=0$, $T_{2N+1}=1$ leads to $T_0 = E_{2N+1}/E_0$.

The phase of each polarization and their phase difference are calculated as follows:

$$\phi_{s,p} = \tan^{-1}\left(\frac{\mathrm{Im}(T_0^{s,p})}{\mathrm{Re}(T_0^{s,p})}\right)$$

and $\Delta\phi = \phi_s - \phi_p$.

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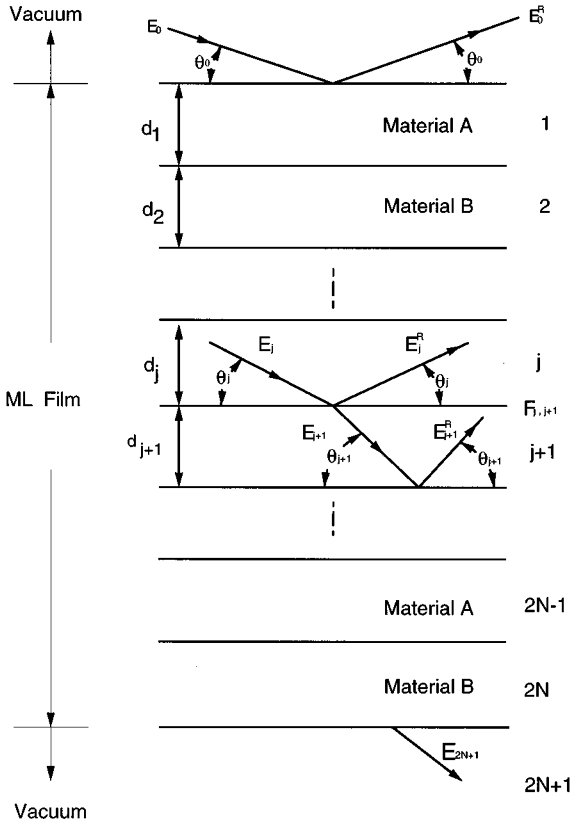

FIG. 1. Electric fields in a multilayer.

In our calculation, the index of refraction in the soft x-ray spectral region was evaluated using the atomic scattering data of Henke.[14]

III. TRANSMISSION PHASE CHARACTERISTICS

Figure 2 shows a typical transmission characteristics of a ML. The calculation was done for a Rh/Si ML at a wavelength of 13 nm. This ML is composed of 11 bilayers with the thickness d of 10.27 nm. The thicknesses of Rh and Si layer are $d_{\mathrm{Rh}}=0.33d$, $d_{\mathrm{Si}}=0.67d$, respectively. For this ML at this wavelength, the position of the first Bragg peak is $\theta \simeq 40°$. The maximum phase difference takes place near the Bragg angle and the critical angle (around 15°) with a drastic change.

At the critical angle, the phase difference is large but the transmittance is too low for any useful purpose. At the Bragg angle, the phase difference is larger than 90°. At $\theta=38.8°$, $\Delta\phi/180°$ becomes close to -0.5 with transmittance of a few tens of percents. This can be utilized as a quarter-wave plate.

For a given number of bilayers, a phase difference as large as possible is helpful in designing a quarter-wave plate. In order to obtain a large phase difference, the selection of materials should be addressed before one starts to find an optimum structure for a quarter-wave plate. For this purpose the criterion for the maximum reflectivity has been used but there is no reason that it should hold for the maximum phase difference between transmitted s- and p-polarized beams as well.

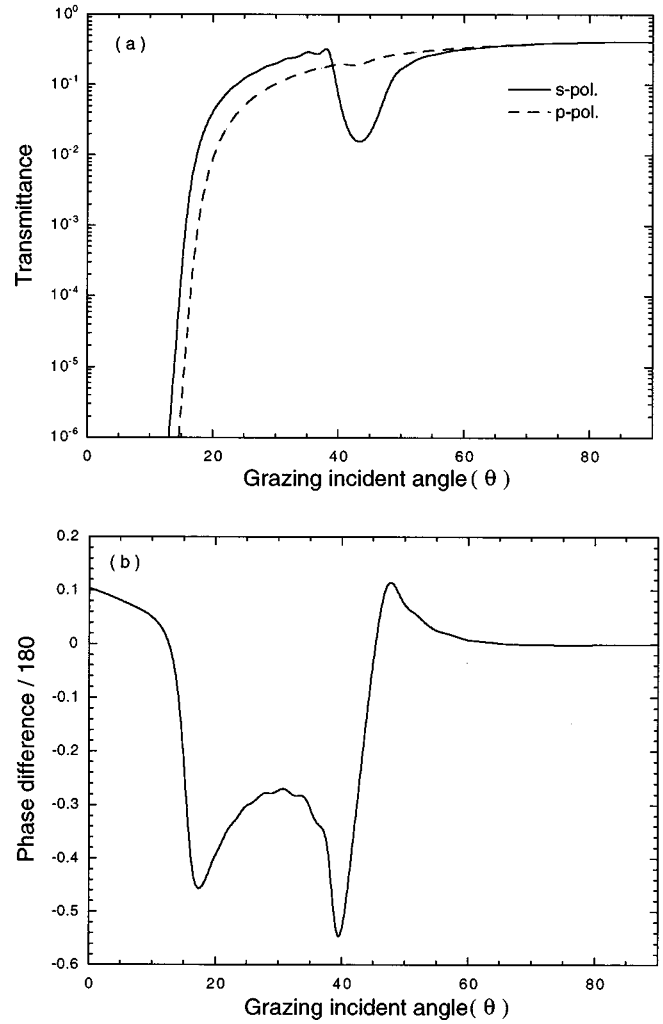

FIG. 2. (a) Calculated transmittances for the s- and p-polarized beams. (b) Relative phase difference between two polarized beams for Rh/Si ML at $\lambda = 13$ nm.

Consider a single interface between two media with different refractive indices. The complex transmission coefficients of s- and p-polarized beam t_s and t_p, respectively, at the interface is given by[15]

$$t_s=\frac{2n_1 \sin\theta_1}{n_1 \sin\theta_1+n_2 \sin\theta_2}=\frac{2n \sin\theta_1}{n \sin\theta_1+\sin\theta_2}, \tag{2}$$

$$t_p=\frac{2n_1 \sin\theta_1}{n_2 \sin\theta_1+n_1 \sin\theta_2}=\frac{2n \sin\theta_1}{\sin\theta_1+n \sin\theta_2}, \tag{3}$$

where

$$n_1=1-\delta_1-i\beta_1, \quad n_2=1-\delta_2-i\beta_2, \tag{4}$$

$$n=\frac{n_1}{n_2}=\frac{1-\delta_1-i\beta_1}{1-\delta_2-i\beta_2}\equiv\Delta-i\beta \tag{5}$$

with

$$\Delta\equiv\frac{1-\delta_1}{1-\delta_2} \quad \text{and} \quad \beta\equiv\frac{1-\delta_1}{1-\delta_2}\left(\frac{\beta_1}{1-\delta_1}-\frac{\beta_2}{1-\delta_2}\right).$$

TABLE I. Structural parameters of several multilayers for the maximum phase difference at $\lambda=13$ nm. The number of bilayers is 20 and the grazing angle of incidence around 50°. This table also shows the transmittances of the s- and p-polarized lights and their phase difference. The terms $1-\delta$ and β are the real and imaginary part of the index of refraction, respectively.

M_1[a]	M_2[b]	Angle(°)[c]	d(nm)[d]	γ[e]	T_s	T_p	$\Delta\phi/180$	$\left\lvert \frac{\beta_1}{1-\delta_1} - \frac{\beta_2}{1-\delta_2} \right\rvert \times 10^3$
Rh	Si	49.9	8.765	0.4825	0.0147	0.0552	−0.8894	26.164
Rh	Sr	49.9	8.925	0.4825	0.0153	0.0481	−0.7651	25.393
Rh	Be	50.0	8.885	0.4825	0.0126	0.0473	−0.7766	25.104
Ru	Si	49.9	8.745	0.5050	0.0375	0.1829	−0.7533	14.234
Ru	Sr	50.0	8.885	0.5050	0.0407	0.1643	−0.6224	13.463
Ru	Be	49.9	8.865	0.5050	0.0368	0.1591	−0.6390	13.174
Mo	Si	50.0	8.625	0.5050	0.1341	0.4433	−0.4495	6.328
Mo	Sr	50.0	8.765	0.5050	0.1569	0.4022	−0.3337	5.557
Mo	Be	49.9	8.745	0.5050	0.1434	0.3900	−0.3508	5.268
Nb	Si	49.9	8.585	0.5050	0.2248	0.5684	−0.3360	4.047
Nb	Sr	49.9	8.725	0.5050	0.2539	0.5177	−0.2288	3.275
Nb	Be	49.9	8.685	0.5050	0.2243	0.5031	−0.2417	2.986

[a]High-Z element.
[b]Low-Z element.
[c]The grazing angle of incidence.
[d]Bilayer thickness.
[e]Ratio of thickness of high-Z element layer to bilayer thickness.

Since $1-\delta_1 \gg \beta_1$ and $1-\delta_2 \gg \beta_2$, β_1^2 and β_2^2 are neglected. Thus, $\Delta \gg \beta$. Using Snell's law, one can obtain

$$\tan\phi_s \simeq \frac{-\beta}{\Delta\sqrt{1-\Delta^2\cos\theta_1}(\Delta\sin\theta_1+\sqrt{1-\Delta^2\cos\theta_1})}, \quad (6)$$

$$\tan\phi_p \simeq \frac{-\beta(\sin\theta_1\sqrt{1-\Delta^2\cos\theta_1}+\Delta^3\cos^2\theta_1)}{\Delta\sqrt{1-\Delta^2\cos\theta_1}(\sin\theta_1+\Delta\sqrt{1-\Delta^2\cos\theta_1})}. \quad (7)$$

Hence,

$$\tan\Delta\phi = \tan(\phi_s-\phi_p) \simeq \tan\phi_s - \tan\phi_p = \frac{-\beta(1-\Delta^2)\cos^2\theta_1(\sqrt{1-\Delta^2\cos\theta_1}-\Delta\sin\theta_1)}{\sqrt{1-\Delta^2\cos\theta_1}(\sin\theta_1+\Delta\sqrt{1-\Delta^2\cos\theta_1})(\Delta\sin\theta_1+\sqrt{1-\Delta^2\cos\theta_1})}. \quad (8)$$

To obtain a large phase difference, $|\tan\Delta\phi|$ should be as large as possible. Considering that the magnitude of cosine and sine is of the order of unity, the magnitude of $\tan\Delta\phi$ would be determined by $\beta(1-\Delta^2)$ for a given angle. For a large absolute value of $\tan\Delta\phi$, the absolute value of $\beta(1-\Delta^2)$ should be large. This implies that if we select two materials for which the difference in the real parts of the refractive indices and $|[\beta_1/(1-\delta_1)]-[\beta_2/(1-\delta_2)]|$ are large, one can obtain a significant phase difference. This result is for a single interface but turns out to be true for a ML as discussed below.

Table I shows the maximum phase difference at 13 nm (95.4 eV) for several MLs with 20 bilayers at a Bragg angle of 50°. For each pair of materials, the structural parameters d (bilayer thickness) and γ (the ratio of the thickness of high-Z element to d) were numerically examined to yield the largest phase difference for given conditions of $N=20$, $\lambda=13$ nm and the grazing angle of incidence of 50°. The last column of this table shows the values of $|[\beta_1/(1-\delta_1)]-[\beta_2/(1-\delta_2)]|$ for each pair of materials. Note that the larger this value is, the larger the phase difference is, as expected by the result from a single interface.

One of the factors which affect the phase difference is the angle of incidence of the incoming beam. As shown in Fig. 2 and described in Ref. 5, a significant phase difference is expected when the angle of incidence is near Bragg angle of a ML structure. To investigate how the grazing angle of incidence changes the maximum phase difference, a series of computer simulations has been done to find out the structural parameters (d and γ) which yield the maximum phase difference for a given grazing angle of incidence. The calculations were done at the wavelength of 13 nm for Rh/Si ML with 20 bilayers. The grazing angle of incidence was changed from 30° to 70° by a step of 10°. The parameter

TABLE II. Grazing angle of incidence vs the maximum phase difference for Rh/Si ML. $N=20$ and $\lambda=13$ nm.

$\theta(°)$	d(nm)	γ	T_s	T_p	$\Delta\phi/180$
30.0	14.00	0.4825	0.0001	0.0003	−2.2122
39.8	10.71	0.5050	0.0014	0.0090	−1.4129
49.9	8.765	0.4825	0.0147	0.0552	−0.8894
59.7	7.666	0.4825	0.0619	0.1178	−0.5161
69.4	6.997	0.4825	0.1534	0.1827	−0.2384

scan in d and γ space with the restriction of Bragg condition being satisfied was done for the maximum phase difference at a given angle. The results are shown in Table II. Note that the maximum phase difference becomes large as the grazing angle of incidence become smaller. However, the transmission behaves in the opposite way. It is because the light has to go through a longer path as the grazing angle of incidence decreases. The thickness ratio also affects the phase difference. With $N=20$, $\theta\simeq 50°$ and $\lambda=13$ nm for Rh/Si ML, the bilayer thickness for the maximum phase difference was found for each thickness ratio, γ, from 0.1 to 0.9 by a step of 0.1. Table III shows that for γ less than around 0.5, the maximum phase difference also increases as γ increases but for γ larger than 0.5, the maximum phase difference becomes smaller. The transmission, however, monotonically decreases as γ increases. At both extreme values of γ, for example, $\gamma=0.1$ and 0.9, the amount of one material is so large compared to that of the other that the whole system may not be considered a ML effectively but a bulk of one material. Hence, at both extremes, the maximum phase difference should be small and the optimum value of γ for the maximum phase difference would be around 0.5. Similar behaviors have been observed for other ML systems under this study. The transmission keeps decreasing due to the amount of highly absorbing material increasing with γ.

Figure 3 shows the phase difference as a function of the number of bilayers. The phase difference increases linearly with the number of bilayers. Thus a phase difference and transmittance can be further controlled by the number of bilayers.

TABLE III. Thickness ratio γ vs phase difference for Rh/Si ML with $N=20$ and $\lambda=13$ nm.

d(nm)	γ	$\theta(°)$	T_s	T_p	$\Delta\phi/180$
8.425	0.10	49.8	0.4284	0.5095	−0.1728
8.485	0.20	49.8	0.1708	0.2902	−0.4347
8.545	0.30	49.8	0.0791	0.1642	−0.6802
8.565	0.33	49.9	0.0566	0.1386	−0.7374
8.645	0.40	49.8	0.0351	0.0912	−0.8412
8.885	0.50	49.8	0.0133	0.0490	−0.8935
9.025	0.60	49.6	0.0074	0.0248	−0.8277
9.265	0.70	49.7	0.0044	0.0124	−0.6432
9.465	0.80	50.3	0.0035	0.0065	−0.3757
9.465	0.90	51.7	0.0037	0.0041	−0.1195

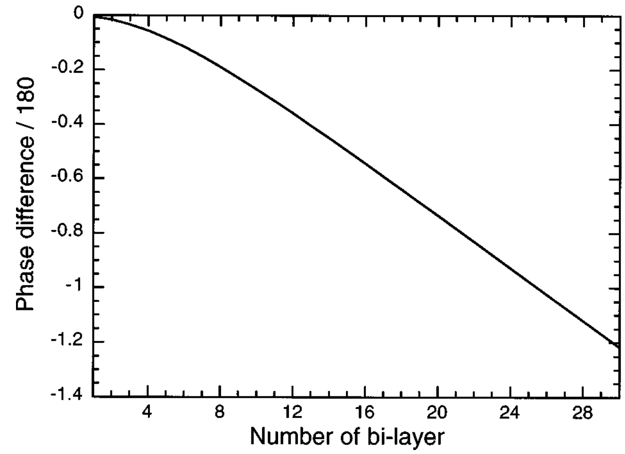

FIG. 3. Phase difference vs the number of bilayers for Rh/Si ML.

IV. SOFT X-RAY TRANSMISSION QUARTER-WAVE PLATE

To be a transmission quarter-wave plate, a ML should yield not only the phase difference of 90° but also a high and equal transmittance for each polarization. Using the effect of various structural parameters on the transmission characteristics of a ML as described in the previous section, we have searched for optimized structural parameters for various ML systems as quarter-wave plates at the wavelengths of 13 and 4.4 nm. Table IV lists several ML systems as quarter-wave plates at 13 nm. For this search, the grazing angle of incidence was chosen to be around 50° for 13 nm and 43° for 4.4 nm, respectively, and the thickness ratio was fixed at 0.33, because reasonable phase difference and transmittance are expected as discussed in Sec. III. Transmittance for each polarization is also shown with their phase difference being very close to 0.5. Almost perfect quarter-wave plates are expected for Rh/Be, Ru/Si, and Ru/Sr MLs. The Rh/Be ML system just needs 11 layers to attain the phase difference of

TABLE IV. Optimized structural parameters as quarter-wave plates. The thickness ratio is fixed at 0.33.

λ(nm)	High Z	Low Z	$\theta(°)$	N	d(nm)	T_s(%)	T_p(%)	$\Delta\phi/180$
13	Rh	Si	48.9	16	8.565	24.3	20.0	−0.506
	Rh	Sr	49.2	17	8.745	15.0	16.0	−0.495
	Rh	Be	49.1	11	8.705	15.4	15.5	−0.495
	Ru	Si	49.2	19	8.525	33.1	33.9	−0.507
	Ru	Sr	49.2	22	8.705	24.8	24.6	−0.494
	Ru	Be	49.2	22	8.665	22.7	23.6	−0.503
	Mo	Si	49.6	29	8.485	40.3	43.8	−0.507
	Mo	Sr	49.8	36	8.645	22.5	29.0	−0.497
	Mo	Be	49.7	37	8.605	20.3	25.9	−0.493
	Nb	Si	49.8	38	8.465	42.6	46.2	−0.508
	Nb	Sr	50.1	49	8.605	20.0	27.8	−0.487
	Nb	Be	49.9	48	8.585	17.1	25.8	−0.483
4.4	Co	K	42.7	110	3.246	8.6	8.9	−0.503
	Cr	K	43.0	166	3.226	11.2	10.4	−0.524
	V	K	43.0	195	3.226	12.4	14.4	−0.496
	Co	C	42.7	132	3.246	3.2	3.3	−0.506
	Cr	C	43.0	193	3.226	3.0	3.5	−0.470

TABLE V. Effect of imperfections at interface on the transmission characteristics. For Rh/Si ML, $N=16$, $d=8.565$ nm, $\gamma=0.33$ at $\lambda=13$ nm and for Co/K ML, $N=110$, $d=3.246$ nm, $\gamma=0.33$ at $\lambda=4.4$ nm.

ML	σ(nm)	$\theta(°)$	T_p/T_s	$\Delta\phi/180$
Rh/Si	0.00	49.7	1.2756	−0.5509
	0.40 (~5% of d)	49.8	1.7558	−0.5228
	0.85 (~10% of d)	50.2	1.4631	−0.4437
	1.30 (~15% of d)	50.8	1.2020	−0.1738
Co/K	0.00	42.8	2.5014	−0.5187
	0.20 (~5% of d)	42.8	1.9041	−0.4805
	0.35 (~10% of d)	42.8	1.3191	−0.3337
	0.50 (~15% of d)	42.9	1.4793	−0.2278

90° but, due to their high absorption, the transmittance is low (15%). Mo/Si and Nb/Si ML systems have better transmittance but demand three or four times more bilayers than the Ru/Be ML system. We have also designed quarter-wave plates at $\lambda=4.4$ nm, carbon K edge, as listed in the lower part of Table IV. There have been studies in this regard, using Cr/C or Co/C, etc., ML.[8,9] The pair of Co and K was chosen according to the criterion presented in Sec. II. The performance of this pair is much better than those of Co/C and Cr/C MLs both in terms of the number of bilayers and transmittance.

So far, all the calculations have been done for ideal multilayers where no imperfection at interfaces exists. But in reality, an interface has always imperfections due to roughness and interdiffusion. To investigate the effect of these imperfections on the transmission characteristics, we have used the Debye-Waller factor[16]

$$\mathrm{DW}=\exp\left[-2\left(\frac{2\pi\sigma\sin\theta}{\lambda}\right)^2\right], \tag{9}$$

where σ is an rms value for the degree of imperfection taking into account both diffusion and roughness, λ the wavelength in the medium and θ the grazing angle of incidence. By multiplying Fresnel coefficients by Debye-Waller factor at each interface, the effect was incorporated into the calculation of transmission coefficient.

Table V shows the change of transmittance and phase for Rh/Si and Co/K ML with the increase of the degree of imperfection. As the imperfection increases, the phase difference becomes smaller. This decrease in the phase difference can be compensated by increasing the number of bilayers at the cost of reduction in transmission. Note that the ratio of the transmittance between the s and p polarization becomes closer to unity, which allows the higher degree of circular polarization. An imperfection of 5% does not seem to change the phase difference much at both wavelengths but a defect of 10% is already large enough to reduce the phase difference significantly. The effect at shorter wavelengths is shown to be larger than at longer wavelengths.

V. CONCLUSION

In this article, we have investigated the transmission characteristics of a ML by simulation with an emphasis on the phase difference between the s and p polarization in the soft x-ray region. We have suggested a new criterion for the selection of material pairs to obtain as large a phase difference as possible. For a large phase difference, the real parts of refractive indices of the two elements should be separated as far as possible, and the imaginary parts should not be too high but $|[\beta_1/(1]-[\delta_1)-\beta_2/(1-\delta_2)]|$ needs to be as large as possible. We have also studied the effect of each ML structure parameter on the phase difference and transmittance and found that the maximum phase difference takes place near the Bragg angle and becomes larger as the Bragg angle position decreases. The maximum phase difference increases linearly with the number of bilayers. There exists an optimum value for the thickness ratio in the trade-off between the transmission and phase difference. Based on these results, optimized structural parameters of several ML systems as quarter-wave plates were searched for, and new and better systems were found compared to others' works.

For nonideal MLs, we have also studied the effect of imperfection at the interface by using an analysis based on the Debye-Waller factor. An imperfection of 10% was shown to be already large enough that the phase difference was reduced significantly. The effect at shorter wavelengths was shown to be larger than at longer wavelengths.

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